Critical Temperature for the Three-Dimensional Ising Ferromagnet with First- and Second- Neighbour Interactions

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ABSTRACT.

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The criticality equation for the Ising ferromagnet is solved by numerical approximation for the three cubic lattices. The Hamiltonian considered contains first and second neighbours interactions and the critical temperature is obtained as a function of the coupling ratio f. The results obtained are within a few percent of those of the series calculations of Dalton and Wood (1969) in the range where they can be compared. The range of f is extended far beyond the limits considered by them.

A simple relation appears to exist between the effective number of neighbours ($z_1 + fz_2$) and the critical temperature. This relation implies an approximate lattice-lattice scaling in three dimensions. It is compared with the corresponding relation obtained from the results of Nath and Frank for the hypercubic lattices.

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1 INTRODUCTION

Frank and Mitran (1977) (to be referred to as FM1) introduced a criticality equation from which they calculated the critical temperature of the three dimensional Ising ferromagnet using cumulant averages and product average decomposition (PAD).

Frank, Cheung and Mouritsen (1982) to be referred to as FCM) rewrote parts of that theory and introduced the so-called i - δ relations which simplified the theory.

The results were close enough to results obtained from series expansions to justify further research in that direction. The theory has since been applied with similar success to the d - dimensional hypercubic lattices by Nath (1983) and to the spin 1 Ising model on the 3 - d cubic lattices by Elofer (1984).

Frank and Nath (1985) obtained a general equation for the PAD by applying it to a Cayley tree for which the PAD is exact. They used that general equation to calculate the critical temperature of the d - dimensional hypercubic Ising ferromagnet, with similar success.

The question then naturally occurs as to whether or not that kind of calculation can be carried out on a model which includes second neighbour interactions; the present work is an attempt to answer that question. For that purpose we generalize,

to include second neighbours i) the criticality equation of FM1, ii) the development, based on the Callen-Suzuki identity, (Callen 1963, Suzuki 1965) made in FCM and iii) the PAD method of Frank and Nath (1985).

In § 2 we give the derivation of the criticality equation, following FCM, including first and second neighbours. That equation will eventually be solved for the critical temperature.

In § 3 the product average decomposition (PAD) method is described and the general PAD equation is derived using a "double" Cayley tree and applied to the Ising model for cubic lattices with first and second neighbour interactions.

In § 4 we describe the numerical method we used to approximate the summations over Brillouin zones.

§ 5 contains a description of the programs.

In § 6, Section 6-1 contains our results for the critical temperature as a function of f for the three cubic lattices as well as the analysis of the global behaviour of kT_c/J as a function of the equivalent number of neighbours $z_1 + fz_2$. In Section 6-2 we compare our results with the available data from Dalton and Wood (1969). Section 6-3 is the closing statement.

2 THEORY: CRITICALITY EQUATION

The theory given here is a rewriting, generalized to include second neighbours, of the theory proposed in FM1, modified in FCM and discussed also in Frank (1983) and Nath (1983).

The Hamiltonian of the system considered is

$$H = -1/2 \sum_{i,j} J_{ij} S_i S_j - \sum_i h_i S_i \qquad (1)$$

where

$$J_{ij} = \begin{cases} J \text{ if } i,j \text{ are first neighbours,} \\ fJ \text{ if } i,j \text{ are second neighbours.} \\ \quad f \text{ is a parameter in the present model;} \\ \quad \text{physically it is the relative value of} \\ \quad \text{the overlap integrals for first and} \\ \quad \text{second neighbour pairs.} \\ 0 \text{ in all other cases.} \end{cases}$$

S_i is the operator representing the z-component of spin at site i, its eigenvalues are $\pm 1/2$. h_i is the (external) magnetic field at site i. The summation indices run over all the lattice sites.

This is the Hamiltonian of the Ising ferromagnet. J is assumed to be positive, and f (to a certain extent as discussed in § 6) can take negative values. A small negative value of f corresponds physically to competing ferro and antiferromagnetic interactions with first and second neighbours spins respectively, the situation remaining ferromagnetic.

To obtain the criticality condition, we consider the Fourier transform of the pair correlation function:

$$G(\vec{k}) = \sum_{\ell} \langle S_i S_\ell \rangle \exp\left[i\vec{k}.(\vec{R}_\ell - \vec{R}_i)\right] \qquad (2)$$

($\langle\ \rangle$ stands for thermal average, $\vec{R}_\ell$ and $\vec{R}_i$ are the position vectors of spins S_ℓ and S_i respectively) which diverges for a second-order phase transition point:

$$G(\vec{k}\to\vec{0}) \to \infty \text{ at } T = T_c \qquad (3)$$

since it is related directly to the magnetic susceptibility (see, e.g., Brout (1965), Nath (1983), Elofer (1984)). The problem is then to obtain an equation containing the temperature and expressing the condition (3). For that purpose we define, following Fränk, Cheung and Mouritsen (1982), the operator associated with site i:

$$O_i \equiv \sum_j J_{ij} S_j + \sum_k J_{ik} S_k \qquad (4)$$

where the sites j are first neighbours of site i and the sites k are second neighbours of site i. O_i can also be written, using f, the ratio of coupling constants for 1st and 2nd neighbours

$$O_i = J \left[\sum_j S_j + f \sum_k S_k\right] \tag{6}$$

O_i appears in the Callen-Suzuki identity (Callen 1963, Suzuki 1965)

$$\langle S_i\{\bar{i}\}\rangle = (1/2)\,\langle\{\bar{i}\}\tanh \beta\,(O_i + h_i)/2\rangle \tag{7}$$

where $\{\bar{i}\}$ is any combination of the S_j not including S_i, and $\beta = 1/k_B T$ where k_B is Boltzmann's constant. One can write, with $h_k \neq 0$ and $\{\bar{i}\} = S_\ell$ in (7)

$$\langle S_i S_\ell\rangle = (1/2)\,\langle S_\ell \tanh \beta O_i/2\rangle \qquad \ell \neq i\ ,$$

so that for general ℓ,

$$\langle S_i S_\ell\rangle = (1/2)\,\langle S_\ell \tanh \beta O_i/2\rangle\,(1-\delta_{i\ell}) + \delta_{i\ell}/4$$

where we have used $\langle S_i^2\rangle = 1/4$ for spin 1/2; $\delta_{i\ell}$ is the Kronecker delta.

Rewriting (8) as:

$$\langle S_i S_\ell\rangle = (1/2)\langle S_\ell \tanh(\beta O_i/2)\rangle - (1/2)\langle S_\ell \tanh(\beta O_i/2)\rangle \delta_{i\ell} + \delta_{i\ell}/4$$

it is noted that in the second term $S_\ell = S_i$.

Using (7) with

$$\{i\} = \tanh\ (\beta O_i/2)$$

one obtains an alternate expression for the second term which contains explicitly only the operator O_i:

$$(1/2)\langle S_i \tanh(\beta O_i/2)\rangle = \langle \tanh^2(\beta O_i/2)\rangle/4$$

so that (8) may be cast in the form

$$\langle S_i S_\ell\rangle = \langle S_\ell \tanh(\beta O_i/2)\rangle/2 + \delta_{i\ell}\langle 1-\tanh^2(\beta_1 O_i/2)\rangle/4$$

or, equivalently,

$$\langle S_i S_\ell\rangle = (1/2)\langle S_\ell \tanh(\beta O_i/2)\rangle + \delta_{i\ell} L \qquad (9)$$

where

$$L = \langle \mathrm{sech}^2(\beta O_i/2)\rangle/4 \qquad (10)$$

and is obviously finite

Using the physical property

$$\langle S_\ell^{2n+1}\rangle \to 0 \quad \text{as } T \to T_c \qquad n = 0, 1, 2, \ldots$$

When there is no external field and, indeed, that the thermal average of the product of any odd number of operators S_j vanishes at or above T_c, we remark that the

$$\langle 0_i^{2n+1} \rangle \qquad n = 0, 1, 2 \ldots$$

also vanish at $T = T_c$

And; by L'Hospital's rule, at $T = T_c$:

$$\lim_{h_j \to 0} \left[\lim_{\substack{h_\ell \to 0 \\ \forall\, \ell \neq j}} \left(\langle 0_i^{2n+1} \rangle / \langle 0_i \rangle \right) \right]$$

(where h_j is the last field to go to zero)

$$= \lim_{h_j \to 0} \left[(\partial / \partial h_j) \lim_{\substack{h_\ell \to 0 \\ \forall\, \ell \neq j}} \langle 0_i^{2n+1} \rangle / (\partial / \partial h_j) \lim_{\substack{h_\ell \to 0 \\ \forall\, \ell \neq j}} \langle 0_i \rangle \right] \tag{11}$$

$$= \lim_{h_j \to 0} \left[\lim_{\substack{h_\ell \to 0 \\ \forall\, \ell \neq j}} \{ \langle S_j\, 0_i^{2n+1} \rangle / \langle S_j\, 0_i \rangle \} \right] = R_n$$

R_n is finite because it is the quotient of finite averages of spin products containing an even number of spins; that is why the limits exists. Moreover we assume that R_n are independent of j and the way the h_ℓ's go to zero.

We are especially interested in

$$\langle S_\ell \tanh(\beta O_i/2)\rangle$$

which appears on the right-hand side of (9). This can be expanded in a series of the form (since tanh is an odd function)

$$\sum_n \alpha_n \langle S_j O_i^{2n+1}\rangle$$

which, by (11) can be written as

$$\langle S_j O_i\rangle \sum_n \alpha_n R_n \text{ is, by (11),}$$

site-independent (in the case of zero external field). Writing this coefficient formally as $2A/J(0)$, the above conclusion is summarized by the statement that A as defined by (12) is site-independent:

$$2A/J(0) = \langle S_\ell \tanh(\beta O_i/2)\rangle / \langle S_\ell O_i\rangle \qquad (12)$$

where $J(0)$ is the space Fourier transform of the exchange integral,

$$J(\vec{k}) = \sum_\ell J_{i\ell} \exp\left[i\vec{k}.(\vec{R}_\ell - \vec{R}_i)\right] \qquad (13)$$

evaluated at the origin:

$$J(0) = J(z_1 + fz_2) \qquad (14)$$

where z_1 is the number of first neighbours of site i and z_2 the the number of second neighbours of site i.

We can write (9), using (12), as

$$\langle S_i S_\ell \rangle = (A/J(0))\langle O_i S_\ell \rangle + \delta_{i\ell} L. \tag{15}$$

Substituting (15) into (2) and using (4) and inserting

$$\exp\,[i\vec{k}.\,(\vec{R}_m - \vec{R}_m)]$$

as a factor, one looks for an equation for $G(\vec{k})$:

$$G(\vec{k}) = \sum_\ell (A/J(0))\langle S_\ell\, 0_i\rangle \exp\,[i\vec{k}.\,(\vec{R}_\ell - \vec{R}_i)]$$

$$+ \sum_\ell \delta_{i\ell} L \exp\,[i\vec{k}.(\vec{R}_\ell - \vec{R}_i)] \tag{16}$$

$$= \sum_{\ell,m} (A/J(0))\langle S_\ell S_m\rangle \exp\,[i\vec{k}.(\vec{R}_\ell - \vec{R}_m)]$$

$$x\, J_{im} \exp\,[i\vec{k}.(\vec{R}_m - \vec{R}_i)]$$

$$+ \sum_\ell \delta_{i\ell} L \exp\,[i\vec{k}.(\vec{R} - \vec{R}_i)] \tag{17}$$

Using (13) (with summation over m) and (2) (with summation over ℓ) we have:

$$G(\vec{k}) = (A/J(0))G(\vec{k})J(\vec{k}) + L \tag{18}$$

or, solving,

$$G(\vec{k}) = L/[\,1 - AJ(\vec{k})/J(0)]\ . \qquad (19)$$

In order to satisfy (3), one has, from (19)

$$A = 1 \text{ at } T = T_c$$

which is the criticality equation.

With (12), the criticality equation is

$$A = J(0)\langle S_\ell \tanh(\beta_c\, O_i/2)\rangle/2\langle S_\ell\, O_i\rangle = 1 \text{ at } T = T_c \qquad (20)$$

Equation (20) is formally the same as the criticality equation of FM1 and of FCM, except that now O_i is defined more generally so as to include second neighbours. A is site independent owing to (11). We can therefore take S_ℓ to be S_i itself or one of its neighbours, first or second. If we choose $S_\ell = S_i$ as in Frank et al (1982), we have, using (7),

$$A = J(0)\langle \tanh^2(\beta_c\, O_i/2)\rangle/2\ \langle O_i\ \tanh(\beta_c\, O_i/2)\rangle = 1 \text{ at } T = T_c \qquad (21)$$

as the criticality equation to be solved for β_c.

We might just as well choose ℓ to be a neighbour of i. Assuming that first and second neighbours are equally valid choices, one may replace S_ℓ in (20) by $O_i/J(0)$ since, for first

neighbours only we would have:

$$S_\ell = O_{i1}/z_1 J \quad , \quad O_{i1} = J \sum_{j=1st} S_j$$

and for the second neighbours only, with fJ coupling,

$$S_\ell = O_{i2}/z_2 fJ \quad , O_{i2} = fJ \sum_{k=2nd} S_k$$

then, using the theorem : if $a/b = c/d = r$, then

$(a + c)/(b + d) = r$ also,

$$S_\ell = (O_{i1} + O_{i2})/(z_1 J + f z_2 J) \equiv O_i/J(0)$$

and we have another criticality equation

$$A' + J(0)\langle O_i \tanh(\beta_c O_i/2)\rangle/\langle O_i^2\rangle = 1 \qquad (22)$$

Both (21) and (22) where considered (separately) in the evaluation of the critical temperature. Although according to the theory they should give identical results, they do not, since the theory is not exact. Hence A is called A' in (22) in order to distinguish the two conditions.

It should be noted that Girvin (1978) pointed out that the choice $\ell = i$ gives more accurate results, and that Frank and Cheung (1984), in their consistent theory, have only the choice $\ell = i$, in the case where nearest neighbours only were considered. In the present work the best results were also obtained with equation (21).

3. SOLUTION OF THE CRITICALITY EQUATION

3 - 1 Definition of T_{2n}

The criticality equations (21) and (22) contain thermal averages of even functions of O_i . To solve the criticality equation for β_c we first consider the expansion

$$\langle f_{even}\ (O_i/J(0))\rangle = \langle \sum_{n=0}^{\infty} a_{2n}\ (O_i/J(0))^{2n} \rangle$$

$$= \sum_{n=0}^{\infty} a_{2n} \langle (O_i/J(0))^{2n} \rangle = a_0 + \sum_{n=1}^{\infty} a_{2n}\ T_{2n} \qquad (23)$$

where $T_{2n} \equiv \langle O_i^{2n} \rangle / J^{2n}(0)$ (24)

In our case $a_0 = 0$ since the even functions in (21) and (22) have the forms:

$$x \tanh x$$

$$\tanh^2 x$$

and x^2

which all vanish as $x \to 0$; therefore

$$\langle f_{even}(O_i/J(0))\rangle = \sum_{n=1}^{\infty} a_{2n}\ T_{2n} \qquad (25)$$

3 - 2 Product average decomposition

The evaluation of thermal averages of even functions of $\frac{O_i}{J(0)}$ amounts to the evaluation of averages of products of spins (see, e.g., (25)).

The product average decomposition (PAD) is a very simple approximation whereby many - spin - product averages are separated into products of pair averages (Frank and Nath (1985)). The PAD enters into the evaluation of the T_{2n} through the following considerations: T_{2n}, when written out explicitely, appears in the form (using (5))

$$T_{2n} = O_i^{2n} / J^{2n}(0) = \langle (\sum_{j=1st} S_j + f \sum_{k=2nd} S_k)^{2n} \rangle / (z_1 + f z_2)^{2n} .$$

Expansion of the right-hand side will generate terms of the form

$$\langle S_{j_1} \text{ --- } S_{j_\ell} \; S_{k_1} \text{ --- } S_{k_m} \rangle \qquad (26)$$

where the j's are first neighbours of i and the k's are second neighbours, $\ell + m = 2n$ and where a particular spin might appear more than once.

The PAD then consists of the following procedure:
i) any spin S_f appearing 2r or 2r + 1 (r>0) times in a

product is replaced by $(\frac{1}{2})^r$ or $(\frac{1}{2})^r S_f$ respectively; when this has been done for all spins appearing more than once, (26) will look like:

$$(\tfrac{1}{2})^p \; < S_{j_1} \text{ --- } S_{j_\ell} \; S_{k_1} \text{ --- } S_{k_m} > \qquad (27)$$

where : $\ell + m + 2p = 2n$. And no spin, now, appears more than once in the average (27).

ii) The product average is decomposed into pair averages:

$$(\tfrac{1}{2})^p \; <S_{j_1} S_{j_2}> <S_{j_3} S_{j_4}> \text{ --- } <S_{k_{m-1}} S_{k_m}> \qquad (28)$$

where three kinds of pair averages can occur:

$$< S_{j_1} S_{j_2} > \; , \; < S_{k_1} S_{k_2} > \text{ and } < S_j S_k >.$$

iii) all pair averages of the term $< S_{j_1} S_{j_2} >$ are replaced by a suitably defined average first neighbour pair average which we call $\bar{p}_{11}$,

$$< S_{j_1} S_{j_2} > = \bar{p}_{11} \qquad (29)$$

b) all pair averages of the form $< S_{k_1} S_{k_2} >$ are replaced by a suitably defined average second neighbour pair average which we call $\bar{p}_{22}$,

$$< S_{k_1} S_{k_2} > = \bar{p}_{22} \qquad (30)$$

c) all pair averages of the form $\langle S_j\ S_k \rangle$ are replaced by a suitably defined average first-second neighbour pair average which we call $\bar{p}_{12}$

$$\langle S_j\ S_k \rangle = \bar{p}_{12} \tag{31}$$

iv) Uniqueness is imposed on the decomposition (28) by the relation

$$\bar{p}_{12} = (\bar{p}_{11}\ \bar{p}_{22})^{\frac{1}{2}} \tag{32}$$

To illustrate how (32) solves the uniqueness problem, we consider for example $\langle S_{j_1}\ S_{j_2}\ S_{j_3}\ S_{k_1}\ S_{k_2}\ S_{k_3} \rangle$. This can be decomposed in essentially two apparently different ways:

$$\langle S_{j_1}\ S_{j_2} \rangle \langle S_{j_3}\ S_{k_1} \rangle \langle S_{k_2}\ S_{k_3} \rangle = \bar{p}_{11}\ \bar{p}_{12}\ \bar{p}_{22}$$

and $$\langle S_{j_1}\ S_{k_1} \rangle \langle S_{j_2}\ S_{k_2} \rangle \langle S_{j_3}\ S_{k_3} \rangle = \bar{p}_{12}^{\,3}$$

The requirement of uniqueness of the decomposition implies that one must have $\bar{p}_{11}\ \bar{p}_{12}\ \bar{p}_{22} = (\bar{p}_{12})^3$ namely, equation (32).

With (32), all PAD decomposition are unique. One needs simply to relate the factor $\sqrt{\bar{p}_{11}}$ to each S_j and the factor $\sqrt{\bar{p}_{22}}$ to each S_k which appears inside a thermal average of the

form (27); i.e., (27) is replaced by

$$(\tfrac{1}{2})^{p} \, (\bar{p}_{11})^{\ell/2} \, (\bar{p}_{22})^{\,m/2} \, .$$

Assuming for the moment that $\bar{p}_{11}$ and $\bar{p}_{22}$ are defined, we now turn our attention to finding a formula which will give T_{2n} and indeed all thermal averages of the desired type (25) as functions of $\bar{p}_{11}$ and $\bar{p}_{22}$.

It will remain only to define $\bar{p}_{11}$ and $\bar{p}_{22}$.

In order to relate the T_{2n} to the $\bar{p}_{\ell\ell}$, we consider a case for which the PAD procedure is exact, namely the case of the system composed of $z_1 + z_2 + 1$ spins and described by the Hamiltonian

$$H_{z_1 + z_2 + 1} = - \sum_{j=1^{st}} J_1 \, S_i \, S_j - \sum_{k=2^{nd}} J_2 \, S_i \, S_k \, . \qquad (33)$$

This is a special case of a Cayley tree. For this system, the spin i is coupled to z_1 (first) neighbours with coupling constant J_1 and z_2 (second) neighbours with coupling constant $J_2 = f J_1$. No other links exist. That the PAD is exact for that case can be seen using the expansions in Appendix A and doing a direct calculation.

To evaluate the thermal averages in that system we need:

$$\exp\left[-\bar{\beta}H_{z_1+z_2+1}\right] = \exp\left[-\bar{\beta}\frac{J_1}{4}\sum_{j=1}^{st} 4S_i S_j - \bar{\beta}\frac{J_2}{4}\sum_{k=2}^{nd} 4S_i S_k\right], \quad (34)$$

where $\bar{\beta}$ is a fictitious "inverse temperature" which is not the inverse critical temperature β_c for the Ising model.

The plan here is to have the $\bar{p}_{\ell\ell}$'s and T_{2n}'s expressed as functions of the intermediate $\bar{\beta}$. Eliminating $\bar{\beta}$ from the two functions, we will then obtain the T's as functions of the P's which is the object of the PAD (see e.g., equation (64)). This procedure is a generalization of the procedure followed by Frank and Nath (1985).

For a particular factor in equation (34), one can expand the exponential $\exp\left[-\bar{\beta}\ (J/4)\ S_i S_\ell\right]$ (with ℓ either a first or a second neighbour of site i)

$$\exp[-\bar{\beta}(J/4)\ 4S_iS_\ell] = 1-\bar{\beta}(J/4)\ S_iS_\ell + \tfrac{1}{2}\ (\bar{\beta}J/4)^2\ (4S_iS_\ell)^2 - \ldots$$

using $4S_iS_\ell = \pm 1$ and thus $(4S_iS_\ell)^{2n} = 1$, and

$$(4S_iS_\ell)^{2n+1} = 4S_iS_\ell,\ n = 1, 2, \ldots$$

we have:

$$\exp[-\bar{\beta}(J/4)\ 4S_iS_\ell] = 1 + \tfrac{1}{2}\ (\bar{\beta}J/4)^2 + (1/24)(\bar{\beta}J/4)^2 + \ldots$$

$$- [\bar{\beta}J/4 + (1/6)(\bar{\beta}J/4)^3 + \ldots]\ 4S_iS_\ell$$

i.e.,

$$\exp[-\bar{\beta}(J/4)\ 4S_iS_\ell] = P - 4QS_iS_\ell$$

where

$$P = \cosh \bar{\beta}J/4 \tag{35}$$

and

$$Q = \sinh \bar{\beta}J/4 \tag{36}$$

Therefore

$$\exp\left[-\bar{\beta}H\frac{z_1}{2} + z_2 + 1\right]$$

$$= \cosh^{\frac{z_1}{2}}(\bar{\beta}J_1/4)\ \cosh^{z_2}(\bar{\beta}J_2/4)$$

$$\times \prod_{j=1}^{\text{st}} [1-4S_iS_j \tanh (\bar{\beta}J_1/4)]$$

$$\times \prod_{k=2}^{\text{nd}} [1-4S_iS_k \tanh (J_2/4)] \tag{37}$$

where $\cosh x + \sinh x = \cosh x\ (1 - \tanh x)$ was used. The following notation will be employed:

$$C_1 = \cosh^{z_1}\left(\bar{\beta}J_1/4\right) \tag{38}$$

$$C_2 = \cosh^{z_2}\left(\bar{\beta}J_2/4\right) \tag{39}$$

$$t_1 = \tanh\left[\bar{\beta}J_1/4\right] \tag{40}$$

$$t_2 = \tanh\left[\bar{\beta}J_2/4\right] \tag{41}$$

Now we have for the averages

$$\langle S_\ell S_m \rangle$$

where ℓ and m are to be taken as the first or second neighbour of site i:

$$\langle S_\ell S_m \rangle = \mathrm{Tr}\left[\exp\left(-\bar{\beta}H_{z_1+z_2+1}\, S_\ell S_m\right)\right] / \mathrm{Tr}\left[\exp\left(-\bar{\beta}H_{z_1+z_2+1}\right)\right]$$

Using (37), (38) and (39)

$$\mathrm{Tr}\left[\exp\left(-\bar{\beta}H_{z_1+z_2+1}\right)\right] = C_1 C_2 \,\mathrm{Tr}\, 1$$

and the average becomes:

$$\langle S_\ell S_m \rangle = (C_1C_2/C_1C_2\mathrm{Tr}1)\,\mathrm{Tr}\{[1-4t_1S_iS_{j_1}] \ldots [1-4t_1S_iS_j]$$

$$\times[1-4t_2S_iS_{k_1}] \ldots [1-4t_2S_iS_k]\, S_\ell S_m\} \tag{42}$$

$= t_1^2/4$ when ℓ and m are both first neighbours of site i

$= t_2^2/4$ when ℓ and m are both second neighbours of site i

$= t_1 t_2/4$ when one of ℓ and m is a first neighbour and the other a second neighbour of site i

Carrying out the trace operations by noting that $\mathrm{Tr}_f\, S_f = 0$ where Tr_f means trace in the subspace of spin f), we obtain

$$\bar{p}_{11} = \langle S_{j_1} S_{j_2} \rangle = (1/4) \tanh^2 (\bar{\beta} J_1/4) \tag{43}$$

$$\bar{p}_{22} = \langle S_{k_1} S_{k_2} \rangle = (1/4) \tanh^2 (\bar{\beta} J_2/4) \tag{44}$$

and

$$\bar{p}_{12} = \langle S_{j_1} S_{k_1} \rangle = (1/4) \tanh (\bar{\beta} J_1/4) \tanh (\bar{\beta} J_2/4) \tag{45}$$

where the j's are first neighbours, the k's second nieghbours of site i:

We remark here that (43)-(45) are consistent with (32) as required.

More convenient that the $\bar{p}_{\ell\ell}$ will be the $q_{\ell\ell}$ defined in terms of them by:

$$q_{11} \equiv 2 (\bar{p}_{11})^{\frac{1}{2}} \tag{46}$$

$$q_{22} \equiv 2 (\bar{p}_{22})^{\frac{1}{2}} \tag{47}$$

from which

$$\exp (\bar{\beta} J_1/4) = [(1 + q_{11})/(1 - q_{11})]^{\frac{1}{2}} \tag{48}$$

$$\exp (\bar{\beta} J_2/4) = [(1 + q_{22})/(1 - q_{22})]^{\frac{1}{2}} \tag{49}$$

In order to evaluate the T_{2n} let us remark that the Hamiltonian (33) can also be written:

$$H_{z_1+z_2+1} = - O_i S_i \tag{50}$$

(with no implied summation over i).

And the thermal average

$$\langle O_i^{2n} \rangle = \mathrm{Tr}\,[\exp(-\bar{\beta} H_{z_1+z_2+1})\, O_i^{2n}] \,/\, \mathrm{Tr}[\exp(-\bar{\beta} H_{z_1+z_2+1})]$$

can be written:

$$\langle O_i^{2n} \rangle = \frac{2^{2n}(\partial^{2n}/\partial \bar{\beta}^{2n})[\mathrm{Tr} \exp(\bar{\beta} O_i S_i)]}{\mathrm{Tr} \exp(\bar{\beta} O_i S_i)} . \tag{51}$$

To work out the traces one can use (5) in the form

$$O_i = J_1 \sum_{j=1}^{z_1 \text{st}} S_j + J_2 \sum_{k=2}^{z_2 \text{nd}} S_k \quad ; \tag{52}$$

using also

$$\exp x = \cosh x + \sinh x = \cosh x\,(1 + \tanh x) \tag{53}$$

one has

$$\mathrm{Tr} \exp(\bar{\beta} O_i S_i)/\mathrm{Tr}\, 1 = \cosh^{z_1}(\bar{\beta} J_1/4)\, \cosh^{z_2}(\bar{\beta} J_2/4) \tag{54}$$

as done in Appendix A. With (54) in (51),

$$\langle O_i^{2n} \rangle = \frac{2^{2n}(\partial^{2n}/\partial\bar{\beta}^{2n})[\cosh^{z_1}(\bar{\beta}J_1/4)\cosh^{z_2}(\bar{\beta}J_2/4)]}{\cosh^{z_1}(\bar{\beta}J_1/4)\cosh^{z_2}(\bar{\beta}J_2\,4)} \qquad (55)$$

To carry out the differentiation one uses

$$\cosh^z(\bar{\beta}J/4) = [(1/2)(\exp(\bar{\beta}J/4) + \exp(-\bar{\beta}J/4))]^z \qquad (56)$$

where J can be either J_1 or J_2 and z can be either z_1 or z_2; using the binomial expansion one gets (as in Appendix B):

$$\frac{\partial^{2n}}{\partial\bar{\beta}^{2n}}\left[\cosh^{z_1}\frac{\bar{\beta}J_1}{4}\cosh^{z_2}\frac{\bar{\beta}J_2}{4}\right]$$

$$=(1/2^{z_1+z_2})\sum_{\lambda=0}^{z_1}\sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\mu^{z_2}\left[J_1(z_1 - 2\lambda)/4 + J_2(z_2 - 2\mu)/4\right]^{2n}$$

$$\times \exp\bar{\beta}\,[J_1(z_1 - 2\lambda)/4 + J_2(z_2 - 2\mu)/4] \qquad (57)$$

where the C_a^b are the binomial coefficients:

$$C_a^b = \frac{b!}{a!(b-a)!}$$

With (57) in (55) and using (56) for the denominator we get:

$$\langle O_i^{2n} \rangle$$

$$= \frac{2^{2n} \sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\mu^{z_2} [D(\lambda,\mu)]^{2n} \exp[-\bar{\beta}D(\lambda,\mu)]}{\sum_{\delta=0}^{z_1} \sum_{\varepsilon=0}^{z_2} C_\delta^{z_1} C_\varepsilon^{z_2} \exp[-\bar{\beta}D(\delta,\varepsilon)]} \tag{58}$$

where

$$[D(\lambda,\mu)] = [J_1(z_1 - 2\lambda)/4 + J_2(z_2 - 2\mu)/4] . \tag{59}$$

And so the T_{2n} (from (24) and (14) are given by

$$T_{2n} = \frac{2^{2n} \sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\mu^{z_2} [D(\lambda,\mu)]^{2n} \exp[-\bar{\beta}D(\lambda,\mu)]}{(z_1J_1+z_2J_2)^{2n} \sum_{\delta=0}^{z_1} \sum_{\varepsilon=0}^{z_2} C_\delta^{z_1} C_\varepsilon^{z_2} \exp[-\bar{\beta}D(\delta,\varepsilon)]} \tag{60}$$

Now we want to eliminate $\bar{\beta}$ of the theory; for that purpose we will use (48) and (49). The idea is the following; (48) and (49) give q_{11} and q_{22} as functions of $\bar{\beta}J_1$ and $\bar{\beta}J_2$ respectively; (60) together with (59) give T_{2n} as a function of $\bar{\beta}J_1$ and $\bar{\beta}J_2$. Therefore T_{2n} can be written as a function of q_{11} and q_{22}. Substitution of (48) and (49) into (60), using also

(59) leads to the first PAD result:

$$T_{2n} = \frac{2^{2n} \sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\lambda^{z_2} [D(\lambda,\mu)] [E(\lambda,\mu)]}{(z_1 J_1 + z_2 J_2)^{2n} \sum_{\delta=0}^{z_1} \sum_{\varepsilon=0}^{z_2} C_\delta^{z_1} C_\mu^{z_2} [E(\delta,\varepsilon)]} \qquad (61)$$

where

$$E(\lambda,\mu) = [(1-q_{11})/(1+q_{11})]^{(z_1/2)-\lambda} [(1-q_{22})/(1+q_{22})]^{(z_2/2)-\mu}$$

Noticing that the denominator involves a binomial expansion, a simplification can be effected (details are in Appendix C):

$$T_{2n} = 2^{-(z_1+z_2)} \sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\mu^{z_2} [2D(\lambda,\mu)/z_1 J_1 + z_2 J_2)]^{2n}$$

$$x\ (1-q_{11})^{z_1-\lambda}\ (1+q_{11})^{\lambda}\ (1-q_{22})^{z_2-\mu}\ (1+q_{22})^{\mu} \qquad (62)$$

It will now be shown how (62) can be generalized to yield a formula valid for any even function of the O_i. Using (62) in (25) and interchanging the summations over λ,μ and n, we have:

$$\langle f_{even}\ (O_i/J(0)) \rangle$$

$$= 2^{-(z_1+z_2)} \sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} \left[C_\lambda^{z_1} C_\mu^{z_2}\ (1-q_{11})^{z_1-\lambda}\ (1+q_{22})^{z_2-\mu}\ (1+q_{11})^{\mu} \right.$$

$$\left. x \sum_{n=1}^{\infty} a_{2n}\ [2D(\lambda,\mu)/(z_1 J_1 + z_2 J_2)]^{2n} \right] \qquad (63)$$

which is, again using (25) formally,

$$\langle f_{even}\,(0_i/J(0))\rangle = 2^{-(z_1+z_2)} \sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} C_\lambda^{z_1}\, C_\mu^{z_2}$$

$$x(1-q_{11})^{z_1-\lambda}(1+q_{11})^{\lambda}(1-q_{22})^{z_2-\mu}(1+q_{22})^{\mu}\, f_{even}\left[2D(\lambda,\mu)/(z_1J_1+z_2J_2)\right]. \tag{64}$$

This is the fundamental PAD result. It is independent of the Hamiltonian $H_{z_1+z_2+1}$ used in its derivation; any system for which the PAD is used will have (64) as true. Only the q_{11} and q_{22} will depend precisely which system one is considering. In the following section are given the forms taken by the criticality equations under PAD approximation. In the succeeding section we address ourselves to the calculation of the q's for the Ising model with first and second neighbours interactions.

3 - 3 CRITICALITY EQUATIONS WITH PAD

Using (64) in the criticality equation (21) (see Appendix D for details) one has:

$$\sum_{\lambda=0}^{z_1}\sum_{\mu=0}^{z_2}\left[Q(\lambda,\mu)\,\tanh\left[\beta_c\frac{J}{4}\,C(\lambda,\mu)\right] \right.$$

$$\left. x\left[\,\tanh\left(\beta_c\,\frac{J}{4}\,C(\lambda,\mu)\right) - C(\lambda,\mu)/(z_1+fz_2)\right]\right] = 0 \qquad (65)$$

where:

$$Q(\lambda,\mu) = C_\lambda^{z_1}\, C_\mu^{z_2}\,(1-q_{11})^{z_1-\lambda}\,(1+q_{11})^{\lambda}\,(1-q_{22})^{z_2-\mu}\,(1+q_{22})^{\mu} \qquad (66)$$

$$C(\lambda,\mu) = z_1-2\lambda + (z_2-2\mu)\,f \qquad (67)$$

Or, with (64) in (22) see Appendix E for details:

$$\sum_{\lambda=0}^{z_1}\sum_{\mu=0}^{z_2} Q(\lambda,\mu)\,C(\lambda,\mu)\left[\tanh\left(\beta_c J C(\lambda,\mu)/4\right) - C(\lambda,\mu)/(z_1+fz_2)\right] = 0 \qquad (68)$$

Equations (65) and (68) are to be solved for β_c numerically by the Newton-Raphson secant procedure (e.g., Fröberg 1969). For that purpose we still need to know q_{11} and q_{22}; they will be obtained from lattice Green's functions.

3 - 4 LATTICE GREEN'S FUNCTIONS AND THE Q's

To evaluate the $q_{\ell\ell}$'s let us consider T_{2n} with n=1, by (24) and (4):

$$T_2 = \langle \Big(\sum_{\ell'} J_{i\ell'} S_{\ell'} + \sum_{m'} J_{im'} S_{m'} \Big) \rangle / J^2(0) \tag{69}$$

where ℓ' and m' run over first and second neighbours respectively of site i. It is also:

$$T_2 = (1/J^2(0)) \sum_{\ell} \sum_{m} J_{i\ell} J_{im} \langle S_\ell S_m \rangle \tag{70}$$

Where ℓ, m run over all sites. Using the Fourier transform of the pair correlation function (2):

$$\langle S_\ell S_m \rangle = (1/N) \sum_{\vec{k}} G(\vec{k}') \exp [- i\vec{k}'.(\vec{R}_m - \vec{R}_\ell)] \tag{71}$$

(N is the total number of sites in the lattice) and introducing $\exp [i\vec{k}: (\vec{R}_i - \vec{R}_i)] = 1$, (70) becomes

$$T_2 = (1/NJ^2(0)) \sum_{\vec{k}'} \sum_{\vec{\ell}} J_{i\ell} \exp [i\vec{k}: (\vec{R}_i - \vec{R}_\ell)]$$

$$\times \sum_{m} J_{im} G(\vec{k}') \exp [i\vec{k}: (\vec{R}_m - \vec{R}_i)] . \tag{72}$$

The last two summations are recognized to be $J(\vec{k})$, the Fourier transform of the exchange integral (see equation (13) and so

$$T_2 = (1/N) \sum_{\vec{k}'} G(\vec{k}') J^2(\vec{k}')/J^2(0) \qquad (73)$$

where $G(\vec{k})$ is given by (19).

We introduce now the temperature independent k' space summations (Green's functions) that can be evaluated directly from the lattice characteristics and the exchange integrals (explicit forms of the lattice Green's functions discussed here are derived in Appendix F for the cubic lattices):

$$F = (1/N) \sum_{\vec{k}} [1 - J(\vec{k})/J(0)]^{-1} \qquad (74)$$

where $\vec{k}$ runs over all points in reciprocal lattice vector space. Then, using (19) (with A=1), we obtain

$$(1/N) \sum_{\vec{k}} G(\vec{k}) = (L/N) \sum_{\vec{k}} [1 - J(\vec{k})/J(0)]^{-1} = LF \qquad (75)$$

which gives, for L,

$$L = (1/FN) \sum_{\vec{k}} G(\vec{k}). \qquad (76)$$

$\sum_{\vec{k}} G(\vec{k})$ can be obtained from the converse of (2):

$$\langle S_i S_\ell \rangle = \frac{1}{N} \sum_{\vec{k}} G(\vec{k}) \exp [i\vec{k}. (\vec{R}_\ell - \vec{R}_i)] ; \qquad (77)$$

in the particular case $\ell = i$ we have

$$\sum_{\vec{k}} G(\vec{k}) = N/4 \qquad (78)$$

whereby, from (76)

$$L = 1/4F \qquad (79)$$

and thus, from (19),

$$G(\vec{k}) = [4F\,(1-J\,(\vec{k})/J(0)]^{-1} \qquad (80)$$

Using (80) in (73):

$$T_2 = (1/4FN) \sum_{\vec{k}'} (J^2(\vec{k}')/J^2(0))[1-J(\vec{k}')/J(0)]^{-1} \qquad (81)$$

and

$$J^2(\vec{k}')/J^2(0)=(J^2(\vec{k}')/J^2(0)-1+1=[(J(\vec{k}')/J(0))-1][(J(\vec{k}')/J(0)+1]+1$$

we can write

$$T_2=(1/4FN)\ -\sum_{\vec{k}'} [(J(\vec{k}')/J(0))+1] + \sum_{\vec{k}'} [1-J(\vec{k})/J(0)]^{-1}$$

the second summation being F itself:

$$T_2= (1/4FN)\left[(-/J(0)) \sum_{\vec{k}'} J(\vec{k}') - \sum_{\vec{k}'} 1 + F\right]$$

noticing that

$$\sum_{\vec{k}'} J(\vec{k}') = \sum_{\vec{k}'} \sum_{\ell} J_{i\ell}\ \exp\,[i\vec{k}'.\,(\vec{R}_\ell-\vec{R}_i)]$$

$$= \sum_{\ell} J_{i\ell} \sum_{\vec{k}'} \exp\left[i\vec{k}'\cdot(\vec{R}_\ell - \vec{R}_i)\right] = \sum_{\ell} J_{i\ell} N\delta_{i\ell} \mathring{N} J_{ii} = 0$$

by definition of the exchange integral; and

$$(1/N) \sum_{\vec{k}'} 1 = 1$$

we are left with

$$T_2 = (1/4)[1-(1/F)] \quad . \tag{82}$$

F can be evaluated from lattice considerations only (see, for examples, Appendix F); Therefore T_2 is known.

In analogy with (69) we define:

$$T_{2\ \text{near}} \equiv \langle \left(\sum_{j=1st} J_{ij}\ S_j \right)^2 \rangle / (z_1 J_1)^2$$

and

$$T_{2\ \text{next}} \equiv \langle \left(\sum_{k=2nd} J_{ik}\ S_k \right)^2 \rangle / (z_2 J_2)^2$$

Which, after a treatment similar to the one leading to (73), can be written:

$$T_{2\ \text{near}} = \frac{1}{N} \sum_{\vec{k}} G(\vec{k})\ J_1^2\ (\vec{k}) / J_1^2\ (0) \tag{83}$$

$$T_{2\ \text{next}} = \frac{1}{N} \sum_{\vec{k}} G(\vec{k})\ J_2^2\ (\vec{k}) / J_2^2\ (0) \tag{84}$$

where $J_1(\vec{k}) = \sum_{j=1st} J \exp[i\vec{k}.(\vec{R}_j - \vec{R}_i)]$ (85)

and $J_2(\vec{k}) = \sum_{j=2nd} fJ \exp[i\vec{k}.(\vec{R}_k - \vec{R}_i)]$ (86)

Using (80) in (83) we have:

$$T_{2_{near}} = (1/N) \sum_{\vec{k}'} (J_1^2(\vec{k})/z_1^2 J_1^2)[4F(1 - J(\vec{k})/J(0))]^{-1} \quad (87)$$

$$T_{2_{next}} = (1/N) \sum_{\vec{k}'} (J_2^2(\vec{k})/z_2^2 J_2^2)[4F(1-J(\vec{k})/J(0))]^{-1} \quad (88)$$

On the other hand, the T_2's can be related to the $\bar{p}_{\ell\ell}$ in the following manner, starting with (24) and (6):

$$T_2 = \frac{\langle (\sum_{j=1st} S_j + f \sum_{k=2nd} S_k)(\sum_{j'=1st} S_{j'} + \sum_{k'=2nd} S_{k'})\rangle}{(z_1 + f z_2)^2} \quad (89)$$

where j, j' run over the first neighbours of i and k, k' over the second neighbours.

$$= \frac{\sum_{j,j'=1st}\langle S_j S_{j'}\rangle + f^2 \sum_{k,k'=2nd}\langle S_k S_{k'}\rangle + 2f \sum_{j=1st}\sum_{k=2nd}\langle S_j S_k\rangle}{(z_1 + fz_2)^2} \quad (90)$$

In the first summations there are z_1 products where

$$j = j' \text{ and } \langle S_j S_{j'} \rangle = \langle S_j^2 \rangle = \tfrac{1}{4} \tag{91}$$

and $z_1(z_1 - 1)$ products where $j \neq j'$

consequently:

$$\sum_{j,j'=1st} \langle S_j S_{j'} \rangle = z_1 \tfrac{1}{4} + z_1(z_1 - 1)\, \bar{p}_{11} \tag{92}$$

and similarly for the second summations:

$$\sum_{k,k'=2nd} \langle S_k S_{k'} \rangle = z_2 \tfrac{1}{4} + z_2\,(z_2 - 1)\, \bar{p}_{22} \tag{93}$$

The third summations contain $z_1 z_2$ products of a first and a second neighbour spin operator, therefore:

$$\sum_{j=1st} \sum_{k=2nd} \langle S_j S_k \rangle = z_1\, z_2\, \bar{p}_{22} \tag{94}$$

Collecting (92), (93), (94) using also (32) in (90):

$$T_2 = \frac{\frac{z_1}{4} + z_1(z_1-1)\bar{p}_{11} + f^2\left[\frac{z_2}{4} + z_2(z_2-1)\bar{p}_{22}\right] + 2f z_1 z_2 (\bar{p}_{11}\, \bar{p}_{22})^{\frac{1}{2}}}{(z_1 + f z_2)^2} \tag{95}$$

Which is the relation sought between T_2 and the $\bar{p}$'s (or T_2 and the q's if one uses (46) and (47)).

As we pointed out after equation (82) the q's (or the $\bar{p}_{\ell\ell}$'s) cannot be fixed by (95) alone. Instead of (95), then, we use the following expressions for $\bar{p}_{11}$ and $\bar{p}_{22}$ in terms of $T_{2\ near}$ and $T_{2\ next}$.

If we had first neighbours only we would have, $z_2=0$ in (95):

$$T_2 = (1/4z_1) + (z_1 - 1)\bar{p}_{11}/z_1$$

or, solving for $\bar{p}_{11}$:

$$\bar{p}_{11} = (z_1 T_2 - 1/4)/(z_1 - 1) \qquad (96)$$

For first and second neighbours together, the suitable choice cited in PAD section appears to be, in analogy with (96):

$$\bar{p}_{11} \equiv (z_1\ T_{2\ near} - 1/4)/(z_1 - 1) \qquad (97)$$

and

$$p_{22} \equiv (z_2\ T_{2\ next} - 1/4)/(z_2 - 1) \qquad (98)$$

As the $T_{2\ near}$ and $T_{2\ next}$ can in principle be evaluated using (87) and (88), the $\bar{p}$'s, and consequently the q's, may be known; equations (65) and (68) can then be solved numerically for β_c the only remaining unknown (f is taken as a system parameter, it is not an unknown).

In Chapter 4 we show how the $T_{2\ near}$ and $T_{2\ next}$ are calculated in practice.

We have no guarantee that $\bar{p}_{11}$ and $\bar{p}_{22}$ defined by (97) and (98) will satisfy (95) exactly, and in fact they do satisfy (95) only approximately. The discrepancy can be evaluated, since T_2 can be known using (82) and we can compare (82) with (95) in which we put the values of $\bar{p}_{11}$ and $\bar{p}_{22}$ obtained by (97) and (98). That checking was done and the discrepancy is of the order of a few percent; the details are given in Chapter 6 containing the results.

4. NUMERICAL APPROXIMATION: CHADI-COHEN METHOD

We now describe the method used for the numerical evaluation of F in (74), T_{2near} in (87) and T_{2next} in (88).

The basic idea started with Baldereschi (1973) and was further developed by Chadi and Cohen (1973), whose method we essentially follow here; the method and its applications was reviewed quite extensively in Evarestov and Smirnov (1984).

4 - 1 Basic theory

The method is an approximation to integrals or summations over the Brillouin zone of any periodic function in reciprocal space.

Let $f(\vec{k})$ be a periodic function of wave vector $\vec{k}$ with the periodicity of the reciprocal lattice. $f(\vec{k})$ can be expanded in Fourier series:

$$f(\vec{k}) = \sum_{m=0}^{\infty} a_m \exp\left[i\vec{k}.\vec{R}_m \right] \qquad (100)$$

Since the R_m's belong to a Bravais lattice,

the terms can be grouped according to the magnitude of the R_m's; and we have the so-called symmetrized plane wave expansion:

$$f(\vec{k}) = f_o + \sum_{m=1}^{\infty} f_m A_m(\vec{k}) \qquad (101)$$

where:

$$A_m(\vec{k}) = \sum_{|\vec{R}|=C_m} \exp [\, i\vec{k}.\vec{R} \,] \qquad m=1,2,.. \qquad (102)$$

The summation in (102) runs over all vectors in the same "star" or "shell" C_m . The first few $A_m(\vec{k})$ are given, as examples, in Appendix G, for the three cubic lattices.

The integral of $f(\vec{k})$ over the Brillouin zone is then

$$(\Omega/8\pi^3)\int_{BZ} f(\vec{k})d\vec{k} = f_o + (\Omega/8\pi^3)\sum_{m=1}^{\infty} f_m \int_{BZ} A_m(\vec{k})d\vec{k} = f_o \qquad (103)$$

where Ω is the volume of the unit cell in direct lattice; since (see Appendix D in Ashcroft and Mermin (1976)):

$$\int_{BZ} A_m(\vec{k})\, d\vec{k} = 0 \; . \qquad (104)$$

The problem is reduced to the evaluation of f_o.

We have, for a particular point $\vec{k}_i$ in (101):

$$f_o = f(\vec{k}_i) - \sum_{m=1}^{\infty} f_m A_m(\vec{k}_i) \quad . \qquad (105)$$

The original idea (Baldereschi 1973) was to choose one reciprocal lattice vector $\vec{q}_1^{(1)}$ (the "Baldereschi point") such that the greatest number of terms in the summation in (105) vanish and hope that other terms in the summation are negligible That is very crude; the precision can be increased if, for instance, for some particular points $\vec{q}_i^{(\nu)}$

$$\sum_{i=1}^{n} \alpha_i A_m(\vec{q}_i^{(\nu)}) = 0 \qquad m=1,\ldots,n \qquad (106)$$

where $\sum_{i=1}^{n} \alpha_i = 1$ (α_i are weighting factors to be determined by the symmetry of the lattice under consideration), and ν is what we call the order of the approximation. We can write, multiplying (105) by α_i and summing over i,

$$\sum_{i=1}^{n} \alpha_i f_o = \sum_{i=1}^{n} \alpha_i f(\vec{q}_i^{(\nu)}) - \sum_{i=1}^{n} \alpha_i \sum_{m=1}^{\infty} f_m A_m(\vec{q}_i^{(\nu)}) \quad . \qquad (108)$$

using (106) and (107):

$$f_o = \sum_{i=1}^{n} \alpha_i f(\vec{q}_i^{(\nu)}) - \sum_{m>n}^{\infty} f_m \sum_{i=1}^{n} \alpha_i A_m(\vec{q}_i^{(\nu)}) \quad . \qquad (109)$$

Assuming that the f_m for m>n can be neglected somehow, we have:

$$f_o \cong \sum_{i=1}^{n} \alpha_i \, f(\vec{q}_i^{(\nu)}) \qquad (110)$$

which is the central equation of the method.

The problem is now to provide the so called special points $\vec{q}_i^{(\nu)}$ and their weighting factors $\alpha_i^{(\nu)}$ satisfying (106) and (107). To solve that problem we use a proposition, from Chadi and Cohen (1973): if the first

$$A_m(\vec{k}) = \sum_{|\vec{R}|=C_m} \exp\left[i\vec{k}.\vec{R} \right] = 0 \qquad (111)$$

is satisfied by $\vec{q}_1^{(1)}$ for $m=m_1$ and by $\vec{k}_2$ for $m=m_2$ then the set, consisting of n_T points, obtained by

$$\vec{q}_i^{(2)} = \vec{q}_1^{(1)} + T_i \, \vec{k}_2 \qquad \text{for } i=1,\ldots,n_T \qquad (112)$$

where T_i is any of the group operations of the symmetry of the point $\vec{k}_2$ (i.e. a subset of the cubic point group, see Appendix H for the 3X3 matrices representation of these T_i) satisfies

$$\sum_i \alpha_i \, A_m(\vec{q}_i^{(2)}) = 0 \quad \text{for } m=m_1 \text{ or } m=m_2 \qquad (113)$$

where $\alpha_i = 1 / n_T$.

The proof is: by choice of $\vec{q}_1^{(1)}$, $\vec{k}_2$ we have

$$A_m(\vec{q}_1^{(1)})\ A_m(\vec{k}_2) = 0 \qquad \text{for } m=m_1 \text{ or } m=m_2 \tag{114}$$

that is

$$\Big(\sum_{|\vec{R}|=C_m} \exp\ [\ i\vec{q}_1^{(1)}.\vec{R}\ ]\ \Big)\Big(\sum_{|\vec{R}|=C_m} \exp\ [\ i\vec{k}_2.\vec{R}\ ]\ \Big) = 0 \tag{115}$$

$$m = m_1 \text{ or } m_2$$

which is, by lattice symmetry, equivalent to:

$$\Big(\sum_{|\vec{R}|=C_m} \exp\ [\ i\vec{q}_1^{(1)}.\vec{R}\ ]\ \Big)\ \Big(\sum_{j} \exp\ [\ i\vec{k}_2.(T_j\ \vec{R})\ ]\ \Big) = 0 \tag{116}$$

($\vec{R}$ in the second bracket is any of the vectors belonging to C_m)

where T_j are all symmetry group operations of $\vec{R}$ and j counts the number of these operations:

$$\{\ \vec{R}\ \big|\ |\vec{R}| = C_m\ \} = \{\ T_j\ \vec{R}\ \}\ . \tag{117}$$

But since

$$\vec{k}_2.(T_j\ \vec{R}) = (T_\ell\ \vec{k}_2).\vec{R} \tag{118}$$

with $T_\ell = T_j^{-1}$; and also since $\{\ T_j\ \}$ (or $\{\ T_\ell\ \}$) is a complete group, (116) can be written:

$$\sum_{\ell} \sum_{|\vec{R}|=C_m} \exp\left[i(\vec{q}_1^{(1)} + T_\ell \vec{k}_2).\vec{R} \right] = 0$$

which is, by (111) and (112)

$$\sum_{\ell} A_m(\vec{q}_1^{(1)} + T_\ell \vec{k}_2) = \sum_{\ell} A_m(\vec{q}_\ell^{(2)}) = 0 \qquad (119)$$

which prooves (113).(It looks like α_ℓ=1 in (120), but we choose $\alpha_\ell = 1/n_T$ to satisfy (107): $\Sigma_\ell \alpha_\ell = 1$).

The next stage would be constructed with

$$A_m(\vec{k}_3) = 0 \text{ for } m=m_3.$$

Then, in analogy with (114), one has,

$$\sum_{\ell} A_m(\vec{q}_\ell^{(2)}) A_m(\vec{k}_3) = 0 \quad \text{for } m = m_1 \text{ , } m_2 \text{ or } m_3$$

which, following the same argument as the one going from (114) to (119) leads to:

$$\sum_{j} A_m(\vec{q}_j^{(3)}) = 0$$

where

$$\vec{q}_j^{(3)} = \vec{q}_\ell^{(2)} + T_j \vec{k}_3$$

The complete proof follows by induction and the

general result is:

$$\vec{q}_j^{(\nu+1)} = \vec{q}_\ell^{(\nu)} + T_j \vec{k}_{\nu+1} \qquad (120)$$

4 - 2 The extrapolation

Starting with the Baldereschi point we have a value for f_o. Using the Chadi & Cohen proposition we find some points where we evaluate $f(\vec{k})$ and that give another evaluation of f_o :

Baldereschi ("first order")	1 point	$f_o^{(1)}$
Chadi-Cohen ("second order")	n_1 points	$f_o^{(2)}$
" ("third order")	n_2 n_1 points	$f_o^{(3)}$
"	. . .	.
"	. . .	.

The successive values of f_o can be considered as a function of the inverse of the number n of points and a very good value can be obtained by extrapolating the value of f_o when $(1/n) \to 0$. That is what we did, with a four point extrapolation.

The efficiencies of the direct and the extrapolated Chadi-Cohen method are compared for SC case, in Table 4.1. That table also shows that the approximated value differs from the exact one by a very small fraction of a percent.

The computer times are given for comparison purposes. The computer was the Cyber 170 of the Concordia University computer center.

The same behaviour was obtained for the BCC and FCC lattices thereby confirming the usefulness of the extrapolation.

The discrepancy between our critical temperature and the series' critical temperature cannot be attributed to the extrapolated Chadi-Cohen procedure but rather to the approximations and assumptions that enter the theory (cf. the argument leading to (97) and (98) and also to (65) and (68)).

TABLE 4 - 1

Comparison between the direct and extrapolated Chadi-Cohen method applied to the evaluation of F (for the Simple Cubic lattice (the expression evaluated is : F-11 of Appendix F) with f = 0 (the program involved is FSC The exact result is known in that case: (Appendix L))

F = 1.5163860591... (Watson 1939)

Chadi-Cohen			extrapolated Chadi-Cohen		
Order	F	Computer Time CPU sec	Orders	F	Computer Time CPU sec
1	1.29412	0.005			
2	1.4164	0.007			
3	1,46406	0.011			
4	1.49003	0.035	1,2,3,4	1,51628	0.074
5	1.50335	0.22	2,3,4,5	1.516377	0,279
6	1.50987	1.5	3,4,5,6	1.5163854	1.819
7	1.51313	11.5	4,5,6,7	1.516386014	13.672
8	1.51476	91.5			
9	1.51557	727			

4 - 3 Construction of the schemes

To feed the extrapolated Chadi-Cohen method into a computer one needs formulas to get directly the $\vec{k}_i$ and α_i for a given order. These formulas are here derived. Starting with the first neighbours of the origin:

$$A_i(\vec{k}) = \sum_{R = 1^{st} \text{ neighbour of the origin}} \exp(i\vec{k}.\vec{R}) \qquad (120)$$

one can find $\vec{q}_1^{(1)}$ such that $A_1(\vec{q}_1^{(1)}) = 0$; it is the Baldereschi (or some equivalent) point. Then one has to find some $A_\ell(\vec{k})$ such that $A_\ell(\vec{q}_1^{(1)}) \neq 0$ (it is not necessarily for $\ell = 2$) and find some $\vec{k}_2$ such that

$$A_\ell(\vec{k}_2) = 0 \qquad (121)$$

then construct:

$$\vec{q}_i^{(2)} = \vec{q}_i^{(1)} + T_i\vec{k}_2 \qquad (122)$$

where $\{T_i\}$ is the group operation of the symmetry of the point $\vec{k}_2$ relative to the origin. If some generated $\vec{q}$'s lie outside the first Brillouin zone one brings them back into the first B.Z. by a proper translation. The number of points so obtained in the first Brillouin zone give the weighting factors $q_i^{(\nu)}$.

The set of points $\{q_i^{(\nu)}\}$ and the corresponding $\{\alpha_i^{(\nu)}\}$ can be

generated recursively, with adjunction of new $\vec{k}$'s in (120), and a formula can be obtained for a given lattice.

4-3-1 Simple cubic lattice.

The symmetrized plane waves for the simple cubic lattice are (see. e.g. (102)):

$$A_m(\vec{k}) = \sum_{|R| = C_m} \exp.\ (i\vec{k}.\vec{R}) \qquad (123)$$

Where $\vec{R} = (n_x, n_y, n_z)\ a$

$\vec{k} = (k_n, k_y, k_z)\ 2\pi/a$ (124)

(all n's are integers and k's are rational numbers). Substitution of (124) into the exponentials of (123) gives:

$$\exp\ (i\vec{k}.\vec{R}) = \exp(2\pi i(n_x k_x + n_y k_y + n_z k_z)) \ ; \qquad (125)$$

or, using $\exp\ (i\theta) = \cos\theta + i\sin\theta$:

$$\exp\ (i\vec{k}.\vec{R}) = (\cos 2\pi n_x k_x + i\sin 2\pi n_x k_x)(\cos 2\pi n_y k_y + i\sin 2\pi n_y k_y) \times (\cos 2\pi n_z k_z + i\sin 2\pi n_z k_z) \qquad (126)$$

Noticing that, by the symmetry of the direct lattice, for any product of coordinates $n_\alpha k_\alpha$ (where α stands for x, y or z) there will be a product $-n_\alpha k_\alpha$ such that the sine parts of (126) will cancel in pairs in the summation of (123). We will have to take care of the cosines only. Since according to the scheme we want $A_n(\vec{k})$ to vanish, we will consider the vanishing of all the terms in the summation (123); that requires the vanishing of all terms of the form (126), or, using the notation

$$C_\alpha = \cos 2\pi n_\alpha k_\alpha \ ,$$

$$S_\alpha = i \sin 2\pi n_\alpha k_\alpha \quad \text{for} \quad \alpha = x, y, z$$

we require

$$\sum_{|R|=C_m} (C_x + S_x)(C_y + S_y)(C_z + S_z)$$

$$\sum_{|R|=C_m} (C_xC_yC_z + C_xS_yC_z + S_xC_yC_z + S_xS_yC_z + C_xC_yS_z + C_xS_yS_z + S_xC_yS_z + S_xS_yS_z) = 0$$

All the terms containing a sine f nction will cancel in pairs in the summation and we are left only with

$$C_zC_yC_z = 0 \qquad (127)$$

to be satisfied. The complete derivation of the A_m as function of the k's, for the first few values of m, is done in Appendix G.

We therefore require that at least one of the cosines vanish, but to simplify the manipulation of (120) we will choose, following Chadi and Cohen, to make the 3 cosines vanish together.

For the first three shells (see e.g. Table G-1) with

$\vec{R}_1 = (1,0,0)$, $\vec{R}_2 = (1,1,0)$, $\vec{R}_3 = 1,1,1)$,

the following equations

$$\vec{A}_1(k) = 0 \ , \ \vec{A}_2(k)=0 \ , \ \vec{A}_3(k)=0$$

require, with the choice we made that all three cosines vanish,

$$\text{Cos } 2\pi k_x = \cos 2\pi k_y = \cos 2\pi k_z = 0 \qquad (128)$$

from which one may choose

$$k_x = k_y = k_z = 1/4 \qquad (129)$$

i.e. $\vec{k}_1 = (1/4, 1/4, 1/4)$. (130)

Since $k_x = k_y = k_z = 3/4, 5/4, 7/4, \ldots$

would have been equally valid solutions of (128), we remark that the point (129) of the reciprocal lattice make all $A_m(\vec{k})$, for which the $\vec{R}$ has at least one odd component, vanish also. Thus the choice (129) is in the spirit of Baldereschi's idea (cf. statement following(105)).

The next non-vanishing $A_m(\vec{k})$ we have to care about correspond to the shell where all the coordinates, of the points in the to shell, are even numbers. That is, from Table K-1 (Appendix K), the fourth shell with typical lattice vector:

$$\vec{R} = (2,0,0) \tag{131}$$

The vanishing of $A_4(k)$ requires, using (131) in (127):

$$\cos 2\pi 2k_x = 0 \tag{133}$$

or $$k_x = 1/8 \text{ (in units of } 2\pi/a) \tag{133}$$

with k_y and k_z arbitrary.

Continuing in the all-k-coordinates-equal system, we choose our second point to be:

$$\vec{k}_z = (1/8, 1/8, 1/8). \tag{134}$$

That will also annihilate $a_7(\vec{k})$ (corresponding to the typical vector $\vec{R} = (2,2,0)$) and $A_{11}(\vec{k})$ (corresponding to the typical vector $\vec{R} = (2,2,2)$).

The next non-zero symmetrized plane wave in the present context appears when the coordinates of vectors in the shell are all integer multiples of 4; that is, with typical lattice vectors (135)

$$\vec{R} = (4,0,0)$$

which is the 14^{th} shell,

$$\vec{R} = (4,4,0) \tag{136}$$

which if the 27^{th} shell, and

$$\vec{R} = (4,4,4) \tag{137}$$

which is the 41^{th} shell as can be seen in Table K-1 (Appendix K).

All of them vanish with the choice (in units of $2\pi/a$):

$$\vec{k}_3 = (1/16,1/16,1/16). \tag{138}$$

The next step is the even number 6 in the shell corresponding to

$$\vec{R} = (6,0,0). \tag{139}$$

That shell requires

$$12\pi k_x = \pi/2,\ 3\pi/2,\ \ldots \tag{140}$$

or $k_x = 1/24,3/24,5/24\ldots$.

But $k_x = 3/24 = 1/8$ already exists in $\vec{k}_2$. Therefore all symmetrized plane waves corresponding to direct lattice points with at least one coordinate (in units of a) equal to 6 will vanish.

The next possibly non-vanishing case happens when the typical vector of the shell contains integer multiples of 8 like:

$$\vec{R} = (8,0,0)\ ,\ (8,8,0) \text{ or } (8,8,8)\ . \qquad (141)$$

The corresponding $\vec{k}$ is:

$$\vec{k}_4 = (1/32,1/32,1/32) \qquad (142)$$

The successive $\vec{k}$'s needed thus far to fit the scheme (collecting equations (130), (134), (138) and (142) are listed below:

$$\vec{k}_1 = (1/4,1/4,1/4)$$
$$\vec{k}_2 = (1/8,1/8,1/8)$$
$$\vec{k}_3 = (1/16,1/16,1/16)$$
$$\vec{k}_4 = (1/32,1/32,1/32)$$

We will now construct the $\vec{k}$'s of the successive orders and look for formulas we announced after equation (122)

The first order of approximation is given by

$$\vec{q}_1^{(1)} = \vec{k}_1 = (1/4,1/4,1/4) \qquad (143)$$

alone (Baldereschi 1973).

The second order is given by a set of points $\{\vec{q}_1^{(2)}\}$

generated by $\vec{q}_i^{(1)}$ and $\vec{k}_2$ in (120).
These points $\vec{q}_2^{(2)}$ have coordinates that are odd multiples of 1/8, in units of $2\pi/a$. These odd multiples will not exceed 4 (in fact they are $(1/4) \pm (1/8) = 3/8$ or $1/8$). The generated points will be of the typical forms:

$$(1/8,1/8,1/8)\ ,\ (3/8,1/8,1/8)\ ,\ (3/8,3/8,1/8),\ (3/8,3/8,3/8). \quad (144)$$

In the case of cubic symmetry, if the 3 coordinates are equal there are 8 points related to each other by the symmetry operations they are the vertices of the cube. If two coordinates are equal it is as if one dimension of the cube was different; then, cubic symmetry operations will generate one "enlarged" cube along each axis, or 3 x 8 = 24 vertices in all. And finally, if all 3 coordinates are different there are 48 points related to each other by the whole point group operation (see Appendix K for further explanations)

Consequently there are, by an operation of the cubic symmetry point group:

8 points related to (1/8,1/8,1/8)
24 points related to (3/8,1/8,1/8)
24 points related to (3/8,3/8,1/8)
and 8 points related to (3/8,3/8,3/8).

There are 64 points in all. The weighting factors will be for the second order:

$$\begin{aligned} 8/64 &= 1/8 \text{ for } (1/8,\ 1/8,\ 1/8) \text{ and } (3/8,\ 3/8,\ 3/8) \\ 24/64 &= 3/8 \text{ for } (3/8,\ 1/8,\ 1/8) \text{ and } (3/8,\ 3/8,\ 1/8) \end{aligned} \tag{145}$$

For the next generation (third order), we add $\pm$ 1/16) to the coordinates of the four points (145). An odd number of $1/8 \pm 1/16$ will give an odd number of 1/16; and for the same reasons as those previously stated, the odd number of 1/16 will not exceed 8. We will have points of the form, in units of (1/16 $2\pi/a$, (where the number of symmetrical points is given to the right of each one).

$$\begin{aligned} \vec{q}_i^{(3)} = \quad & (1,\ 1,\ 1) \quad 8 \\ & (3,\ 1,\ 1) \quad 24 \\ & (5,\ 1,\ 1) \quad 24 \\ & (7,\ 1,\ 1) \quad 24 \\ & (1,\ 3,\ 3) \quad 24 \\ & (3,\ 3,\ 3) \quad 8 \\ & (5,\ 3,\ 3) \quad 24 \\ & (7,\ 3,\ 3) \quad 24 \\ & (1,\ 5,\ 5) \quad 24 \\ & (3,\ 5,\ 5) \quad 24 \\ & (5,\ 5,\ 5) \quad 8 \\ & (7,\ 5,\ 5) \quad 24 \\ & (1,\ 3,\ 3) \quad 48 \\ & (1,\ 3,\ 7) \quad 48 \\ & (1,\ 5,\ 7) \quad 48 \\ & (3,\ 5,\ 7) \quad 48 \end{aligned} \tag{146}$$

The total number of points generated is 512. The points with 3 coordinates equal have, here, a weighting factor of 8/512 or 1/64. The points having 2 coordinates equal have weighting factors of 24/512 or 3/64. And the points with 3 different coordinates have weighting factors of 48/512 = 6/64.

We note that $1/4 = (1/2)(1/2^{\nu})$ with $\nu = 1$

$1/8 = (1/2)(1/2^{\nu})$ with $\nu = 2$

$1/16 = (1/2)(1/2^{\nu})$ with $\nu = 3$

and so on.

The coordinates of the reciprocal space vectors in the first Brillouin zone given in (143), (145) and (146) of the simple cubic lattice which fit the Chadi-Cohen scheme are thus given by (in units of $2\pi/a$).

$$\{\vec{q}_i^{(\nu)}\} \quad \{(1/2)(1/2^{\nu})(o_1, o_2, o_3)\}, \nu = 1, 2, 3... \quad (147)$$

where o_1, o_2 and o_3 are odd numbers not exceeding 2^{ν}, and ν is the order of the approximation.

The weighting factors can be generated with the use of the following formula; for order ν, they are given by

$1/8^{\nu-1}$ if the 3 coordinates of $\vec{q}$ are equal

$3/8^{\nu-1}$ if two coordinates of $\vec{q}$ are equal (148)

and $6/8^{\nu-1}$ if the 3 coordinates of $\vec{q}$ are different.

4-3-2 Body Centered Cubic Lattice

Following the same procedure as in the simple cubic case, we start with the point, in units of $2\pi/a$, and with a = 1:

$$\vec{q}_1^{(1)} = \vec{k}_1 \quad (1/2, 1/2, 1/2)$$

satisfying

$$A_1(\vec{k}_1) = 0$$

Where $A_1(\vec{k})$ is equation G-38 of appendix G.

the weighting factor is indeed $\alpha = 1$.

The next order, required by $A_2(\vec{k}_2) = 0$ (Given in G-39), is obtained with (in units of $\frac{2\pi}{a}$) :

$$\vec{k}_2 = (1/4, 1/4, 1/4) \quad .$$

And the vectors generated, using (120) are (in units of $\frac{1}{4} \quad \frac{2\pi}{a}$) :

$$\vec{q}_1^{(1)} + T_i\vec{k}_2 = \begin{matrix} (3, 3, 3) \\ (1, 3, 3) \\ (3, 1, 3) \\ (3, 3, 1) \\ (1, 1, 3) \\ (1, 3, 1) \\ (3, 1, 1) \\ (1, 1, 1). \end{matrix}$$

But here we have a new problem since the first four points are outside the first Brillouin zone. The sum of any two coordinates cannot exceed or equal 1 (in units of $2\pi/a$) for the point to be in

the first Brillouin zone of the BCC lattice. That condition is derived in Appendix I. When the points are brought into the first Brillouin zone by translation (of -1 on two coordinates owing to the spatial arrangement of the zones) they become:

(3, 3, 3) → (3, -1, -1) or, by cubic symmetry:
(1, 3, 3) (3, 1, 1)
(3, 1, 3) → (1, 1, 1).
(3, 3, 1)

And we have only two different points for the first order in BCC; (in units of $2\pi/a$):

$$\vec{q}_{,}(2) = \begin{matrix}(1/4,\ 1/4,\ 1/4) \\ (3/4,\ 1/4,\ 1/4)\end{matrix} \quad \begin{matrix}1/2 \\ 1/2\end{matrix} \quad = \vec{\alpha}_{i}(2) \qquad (149)$$

as previously detained by Chadi and Cohen (1973) and Mignen (1978)

The summetrized plane waves $A_m(\vec{k})$ are vanishing for n = 1 to 7 at the $\vec{q}$'s given in (149). The vanishing of $A_8(\vec{k})$ requires the introduction of (in units of $2\pi/a$):

$$\vec{k}_3 = (1/8,\ 1/8,\ 1/8)$$

and the points generated, using (122), are (in units of $2\pi/a$):

	Status		alter translation
	(3/8, 3/8, 3/8)	out	(5/8, 3/8, 1/8)
	(5/8, 3/8 , 3/8)	in	
	(7/8, 1/8, 3/8)	out	(5/8, 1/8, 1/8)
	(7/8, 3/8, 1/8)	out	(5/8, 1/8, 1/8)
$(3/4, 1/4, 1/4)+T_i(7/8, 1/8, 1/8) =$	(5/8, 1/8, 3/8)	in	
	(5/8, 3/8, 1/8)	in	
	(7/8, 1/8, 1/8)	in	
	(5/8, 1/8, 1/8)	in	

	(3/8, 3/8, 3/8)	in	
	(1/8, 3/8, 3/8)	in	(3/4, 1/8, 1/4)
	(3/8, 1/8, 3/8)	in	
	(3/8, 3/8, 1/8)	in	
$(1/4, 1/4 , 1/4)+T_i(1/8, 1/8, 1/8) =$	(1/8, 1/8, 3/8)	in	
	(1/8, 3/8, 1/8)	in	
	(3/8, 1/8, 1/8)	in	
	(1/8, 1/8, 1/8)	in	

and we have, for the second order, the points (in 1/8) $2\pi/a$ and α's in units of 1/16):

$\vec{a}_i^{(3)}$	$\alpha_i^{(3)}$
(1, 1, 1)	1
(3, 1, 1)	3
(3, 3, 1)	3
(3, 3, 3)	1
(5, 1, 1)	3
(5, 3, 1)	3
(5, 3, 3)	1
(7, 1, 1)	1

(150)

The next generation is required by the $A_n(\vec{k})$ containing cosines of $4k_x$, $4k_y$, $4k_z$; that requires the adjunction of the point

$$\vec{k}_4 = (2\pi/a), (1/16, 1/16, 1/16)$$

to the scheme. Combining $\vec{k}_3$ with the $\vec{k}_2$'s of(150) one obtains, for the third order:

	$\vec{q}_i^{(4)}$ in 1/16 units	Status	α_i 1/128 units
(1/8,1/8,1/8) $+T_i$ (1/16,1/16,1/16) =	(3,3,3)	in BZ	1
(α=1)	(3,3,1)		
	(3,1,3)		
	(1,3,3)		
	(3,1,1)		
	(1,3,1)		3
	(1,1,3)		
	(1,1,1)		
(3/8,1/8,1/8) $+T_i$ (1/16,1/16,1/16) =	(7,3,3)		3
(α=3	(7,3,1)		6
	(7,1,3)		
	(5,3,3)		3
	(7,1,1)		3
	(5,3,1)		6
	(5,1,3)		
	(5,1,1)		3
(3/8,3/8,1/8) $+T_i$ (1/16,1/16,1/16) =	(7,7,3)		3
(α=3)	(7,7,1		3
	(7,5,3)		6
	(5,7,3)		
	(7,5,1)		6
	(5,7,1)		
	(5,5,3)		3
	(5,5,1)		3
(3/8,3/8,3/8) $+T_i$ (1/16,1/16,1/16) =	(7,7,7)		1
(α=1)	(7,7,5)		
	(7,5,7)		3
	(5,5,7)		
	(7,5,5)		3
	(5,7,5)		
	(5,5,7		
	(5,5,5)	in BZ	1

	$\vec{q}_i^{(4)}$ in 1/16 units	status	$\alpha_i^{(4)}$ in 1/128 units
(5/8,1/8,1/8) $+T_i$ (1/16,1/16,1/16) =	(11,3,3)	in	3
(α=3)	(11,3,1)		6
	(11,1,3)		
	(9,3,3)		3
	(11,1,1)		3
	(9,3,1)		6
	(9,1,3)		
	(9,1,1)	in	3
(5/8,3/8,1/8) $+T_i$ (1/16,1/16,1/16) =	(11,7,3)	out	(9,5,3)
(α=3)	(11,7,1)	out	(9,5,1)
	(11,5,3)	surf	3
	(9,7,3)	surf	3
	(11,5,1)	surf	3
	(9,7,1)	surf	3
	(9,5,3)	in	6
	(9,5,1)	in	6
(5/8,3/8,3/8) $+T_i$ (1/16,1/16,1/16) =	(11,7,7)	out	(9,5,7)
(α=1)	(11,7,5)	out	(9,5,5)
	(11,5,7)	out	(9,5,5)
	(9,7,7)	surf	1
	(11,5,5)	surf	1
	(9,7,5)	surf	3
	(9,5,7)	surf	
	(9,5,5)	surf	3
(7/8,1/8,1/8) $+T_i$ (1/16,1/16,1/16) =	(15,3,3)	out	(13,3,1)
(α=1)	(15,3,1)	out	(13,1,1)
	(15,1,3)	out	(13,1,1)
	(13,3,3)	surf	1
	(15,1,1)	surf	1
	(13,3,1)	surf	3
	(13,1,3)	surf	
	(13,1,1)	in	3

The BCC scheme now appears as follows:

1) In units of $2\pi/a$ and for order ($\nu = 1, 2, \ldots$) the $\vec{q}$'s are

$$(1, 2^{\nu}) \quad (o_1, o_2, o_3)$$

Where o_1, o_2 and o_3 are positive odd numbers smaller than $2^{\nu-1}$ and the sum of any two of them shall not exceed $2^{\nu-1}$ (the sum of any two coordinates shall not exceed 1; see Appendix I for details).

2) For $\nu = 1$ the weighting factor is 1.

For $\nu > 1$ the weighting factors are, in units of $(1/2)\ (1/8^{\nu-2})$ (where ν is the order of approximation)

and

a) if the three coordinates are equal $\alpha = 1$

b) if any two coordinates are equal

i) the sum of any two components = 1 $\alpha = 1$

and

ii) otherwise $\alpha = 3$

c) all three components are different

i) sum of any two components = 1 $\alpha = 3$

and

ii) otherwise $\alpha = 6$

Those formulas (147) and (148) correspond exactly to the points given in Chadi-Cohen (1973) and Lin-Chung (1978) and allow one to go to any order in the approximation. But the formulas (147) and (148) are not to be found in these papers.

4-3-3 Face Centered Cubic

For zeroth order $A_1(\vec{k}_1) = 0$ given in G-21 (Appendix G) requires, in units of $\frac{2\pi}{a}$; for $\nu = 1$

$$\vec{q}_1^{(1)} = \vec{k}_1 = (1/2,\ 1/2,\ 1/2) \qquad d = 1$$

Since $A_2(\vec{k}_1)$ does not vanish (see G-23), the next point is $\vec{k}_2$ determined by

$$A_2(\vec{k}_2) = 0$$

It gives, solving (G-23):

$$\vec{k}_2 = (1/3,\ 1/4,\ 1/4).$$

Combined, using (120) they give in units of $\frac{1}{4}\ \frac{2\pi}{a}$):

$$\vec{q}_i^{(2)} = (3,\ 3,\ 3)$$
$$(1,\ 3,\ 3)$$
$$(3,\ 1,\ 3)$$
$$(3,\ 3,\ 1)$$
$$(1,\ 1,\ 3)$$
$$(1,\ 3,\ 1)$$
$$(3,\ 1,\ 1)$$
$$(1,\ 1,\ 1).$$

According to (J-1) and (J-2) (in Appendix J), the first four points lie outside the first Brillouin zone. To bring them back in the first Brillouin zone, a translation of $-2\pi/a$ on each coordinate is required owing to the shape and the spatial arrangement of the Brillouin zones. For $\nu = 2$ there are only two different points after these operations are carried over (in units of $(1/4)\ (2\pi/2)$) for $\nu = 2$:

$$\vec{q}_i^{(2)} = \begin{matrix} (1,\ 1,\ 1) & \alpha = 1/4 \\ (3,\ 1,\ 1) & \alpha = 3/4 \end{matrix} \qquad (151)$$

These two points satisfy

$$A_m(\vec{k}) = 0$$

for m values up to 7. The next order is obtained by the requirement

$$A_8\ (\vec{k}_3) = 0$$

which sets $\vec{k}_3 = (\frac{1}{8},\ \frac{1}{8},\ \frac{1}{8})$ (in units of $\frac{2\pi}{a}$)

as can be seen directly in (G-35) (Appendix G)

The combination, using (120), of $\vec{k}_3$ with the two points (151) previously obtained leads to the third order points (in units of

$(1/8)\ (2\pi/a)$; for $\nu = 3$:

$(2,2,2) + (1,1,1) = (3, 3, 3)$ $\alpha = 1/32$

$(3, 3, 1)$
$(3, 1, 3)$ } 3/32
$(1, 3, 3)$

$(3, 1, 1)$
$(1, 3, 1)$ } 3/32
$(1, 1, 3)$

$(1, 1, 1)$ 1/32

$(6,2,2)+T_i\ (1,1,1) = (7, 3, 3)\ \ (5, 5, 1)$ 3/32

$(7, 3, 1)$
$(7, 1, 3)$ } 6/32

$(5, 3, 3)$ 3/32

$(7, 1, 1)$ 3/32

$(5, 3, 1)$
$(5, 1, 3)$ } 6/32

$(5, 1, 1)$ 3/32

The point (7, 3, 3) lies outside the first Brillouin zone and gives (1, 5, 5) when translated.

The FCC scheme now appears as follows:

1) In units of $2\pi/a$ the coordinates of each of each point are given by

$$\vec{q}_\nu = (1/2^\nu)\ (O_1, O_2, O_3)$$

where O_1, O_2, O_3 are odd numbers not exceeding 2^ν and ν is the order of approximation.

2) For $\nu = 1$ the weighting is 1.
For $\nu > 1$ the weighting factors are, in units of $(1/4)\ (1/8^{\nu-2})$:

1 if the 3 coordinates are equal
3 if two of the coordinates are equal
6 if the 3 coordinates are different

This is partially confirmed by Chadi - Cohen (1973).

5 Description of Programs

As a first step, the Chadi-Cohen method was used to obtain the numerical value of F defined in (74) and given explicitly in Appendix F; (F-11) for the simple cubic lattice, (F-19) for the body centered cubic lattice and (F-25) for the face centered cubic case. The extrapolation was done by fitting a third degree polynomial to four points as described in Section 4-2.

In the second step, the values of F for the corresponding lattices were fed into (87) and (88) where four point extrapolation was again used to evaluate the $\vec{k}$ summations.

Using (97), (98), (46) and (47) the numerical values of the q's were obtained.

These procedures, of the first and second steps, are lattice dependent.

The third step is then to solve (65) and (68) for β_c. That last procedure is a Newton-Raphson secant algorithm (Fröberg 1969) and is lattice independent.

The program names are given in Table 5-1 and their listings are contained in Appendix L.

	PROGRAMS		
LATTICES	SC	BCC	FCC
Evaluation of F	FSC	FBCC	FFCC
Evaluation of the q's	T2SC	T2BCC	T2FCC
Solution of $A^{*} = 1$ (65)		BETAC	
Solution of $A^{-} = 1$ (68)		BETACP	

Table 5-1 Program Names

6. RESULTS AND DISCUSSION

6-1-1 Results

Tables 6-1, 6-2 and 6-3 contain our results for the SC BCC and FCC lattices respectively. The first column is the system parameter f defined just after equation (1), the second column is the equivalent number of neighbours, the third and fourth columns contain $k_B T_c / J = 1/\beta_c J$ obtained from (65) (that is for A=1) and from (68) (that is for A'=1) respectively. The fifth column is T_2 obtained from (82) using (74) (74). The sixth column contains the values of T_2 obtained after knowing $\bar{p}_{11}$ and $\bar{p}_{22}$ by using (95). The last two columns columns are $\bar{p}_{11}$ and $\bar{p}_{22}$ respectively.

According to the large range of f analysed we plotted the data on three graphs with different scales. The curves traced on these graphs are discussed in Section 6-1-3.

Table 6-1

SC lattice

		A=1	A'=1				
f	z_1+fz_2	$1/\beta_c J$	$1/\beta_c J$	T_2	$T_2(\bar{p}_{11},\bar{p}_{22})$	$\bar{p}_{11}$	$\bar{p}_{22}$
-0.06	5.28	0.9595	0.9157	.097034	.099739	.056030	.044698
-0.05	5.40	0.9934	0.9525	.094729	.096856	.055253	.044077
-0.04	5.52	1.0269	0.9886	.092568	.094175	.054537	.043504
-0.03	5.64	1.0602	1.0242	.090539	.091677	.053875	.042972
-0.02	5.76	1.0933	1.0592	.088630	.089347	.053262	.042478
-0.01	5.88	1.1260	1.0938	.086831	.087170	.052692	.042018
-10^{-9}	6.0	1.1586	1.1280	.085134	.085134	.052161	.041588
10^{-9}	6.0	1.1586	1.1280	.085134	.085134	.052161	.041588
0.01	6.12	1.1909	1.1617	.083531	.083228	.051666	.041185
0.02	6.24	1.2230	1.1951	.082015	.081440	.051203	.040807
0.03	6.36	1.2549	1.2282	.080579	.079762	.050769	.040452
0.04	6.48	1.2866	1.2610	.079218	.078185	.050362	.040117
0.05	6.60	1.3181	1.2934	.077926	.076702	.049979	.039802
0.06	6.72	1.3494	1.3256	.076699	.075305	.049619	.039504
0.07	6.84	1.3806	1.3576	.075532	.073989	.049280	.039222
0.08	6.96	1.4116	1.3893	.074422	.072747	.048960	.038954
0.09	7.08	1.4424	1.4208	.073364	.071575	.048657	.038701
0.1	7.2	1.4731	1.4521	.072355	.070467	.048371	.038460
0.2	8.4	1.7732	1.7558	.064411	.062120	.046198	.036589
0.3	9.6	2.0638	2.0477	.059133	.057028	.044842	.035363

0.4	10.8	2.3477	2.3319	.055464	.053764	.043954	.034514
0.5	12	2.6268	2.6107	.052829	.051597	.043356	.033905
0.6	13.2	2.9024	2.8856	.05089	.050123	.042947	.033457
0.7	14.4	3.1753	3.1576	.049434	.049103	.042669	.033123
0.8	15.6	3.4460	3.4272	.048329	.048391	.042483	.032871
0.9	16.8	3.7151	3.6950	.047482	.047893	.042363	.032681
1.0	18	3.9827	3.9613	.046829	.047549	.042293	.032538
2.0	30	6.6183	6.5800	.044932	.047245	.042691	.032287
3.0	42	9.2213	9.1629	.045439	.048147	.043541	.032683
4.0	54	11.812	11.731	.046287	.049036	.044350	.033175
5.0	66	14.394	14.291	.047130	.049805	.045064	.033655
6.0	78	16.971	16.846	.047900	.050462	.045687	.034099
7.0	90	19.545	19.397	.048588	.051029	.046235	.034506
8.0	102	22.117	21.945	.049201	.051522	.046720	.034876
9.0	114	24.686	24.490	.049749	.051957	.047152	.035214
10	126	27.253	27.033	.050241	.052344	.047541	.035523
15	186	40.068	39.727	.052109	.053799	.049029	.036753
20	246	52.860	52.397	.053370	.054782	.050053	.037636
30	366	78.404	77.691	.055009	.056075	.051414	.038850
100	1206	250.9	254.2	.058766	.059176	.054702	.041951
300	3606	764.5	763.4	.060862	.061014	.056639	.043874
400	4806	1018	1008	.061248	.061361	.057002	.044243
1000	12006	2538	2519	.062217	.062254	.057931	.045199
3000	36006	7634	7519	.063094	.063099	.058804	.046112
10000	120006	25640	25000	.063695	.063695	.059417	.046759
30000	360006			.063939	.063939	.059668	.047024

Table 6-2

BCC lattice

		A=1	A'=1				
f	z_1+fz_2	$1/\beta_c J$	$1/\beta_c J$	T_2	$T_2(\bar{p}_{11},\bar{p}_{22})$	$\bar{p}_{11}$	$\bar{p}_{22}$
-0.6	4.4	0.6143	0.3800	.115911	.144410	.041681	.049285
-0.4	5.6	0.9640	0.8770	.090149	.104343	.044761	.042740
-0.3	6.2	1.1372	1.0777	.083046	.091692	.044978	.041247
-0.2	6.6	1.3051	1.2617	.077767	.082461	.045016	.040126
-0.15	7.1	1.3870	1.3490	.075616	.078802	.045004	.039658
-0.1	7.4	1.4675	1.4338	.073723	.075648	.044982	.039239
-0.09	7.46	1.4835	1.4505	.073371	.075070	.044977	.039160
-0.08	7.52	1.4994	1.4670	.073028	.074509	.044972	.039083
-0.07	7.58	1.5152	1.4836	.072693	.073965	.044966	.039007
-0.06	7.64	1.5310	1.5000	.072366	.073435	.044960	.038933
-0.05	7.7	1.5468	1.5163	.072047	.072921	.044954	.038860
-0.04	7.76	1.5625	1.5326	.071735	.072421	.044948	.038789
-0.03	7.82	1.5781	1.5488	.071430	.071935	.044942	.038719
-0.02	7.88	1.5937	1.5649	.071133	.071463	.044936	.038650
-0.01	7.94	1.6093	1.5809	.070842	.071004	.044929	.038582
-10^{-9}	8	1.6245	1.5969	.070558	.070558	.044923	.038516
10^{-9}	8	1.6245	1.5969	.070558	.070558	.044923	.038516
0.01	8.06	1.6402	1.6128	.070280	.070124	.044916	.038451
0.02	8.12	1.6557	1.6286	.070008	.069702	.044910	.038387
0.03	8.18	1.6710	1.6444	.069743	.069291	.044903	.038324

0.04	8.24	1.6864	1.6601	.069483	.068892	.044897	.038263
0.05	8.30	1.7016	1.6757	.069229	.068504	.044890	.038202
0.06	8.36	1.7169	1.6913	.068981	.068126	.044884	.038143
0.07	8.42	1.7321	1.7068	.068738	.067759	.044877	.038084
0.08	8.48	1.7472	1.7223	.068500	.067402	.044870	.038027
0.09	8.54	1.7623	1.7377	.068267	.067054	.044864	.037970
0.1	8.6	1.7774	1.7530	.068040	.066716	.044857	.037915
0.2	9.2	1.9260	1.9036	.066012	.063792	.044795	.037407
0.3	9.8	2.0709	2.0497	.064361	.061554	.044740	.036974
0.4	10.4	2.2129	2.1922	.063008	.059834	.044694	.036600
0.5	11	2.3523	2.3317	.061890	.058511	.044657	.036276
0.6	11.6	2.4895	2.4686	.060963	.057495	.044629	.035993
0.7	12.2	2.6249	2.6035	.060191	.056719	.044609	.035745
0.8	12.8	2.7586	2.7365	.059547	.056131	.044597	.035527
0.9	13.4	2.8909	2.8680	.059009	.055693	.044592	.035334
1.0	14	3.0220	2.9981	.058560	.055375	.044593	.035163
2.0	20	4.2920	4.2544	.056786	.055339	.044827	.034216
3.0	26	5.5246	5.4691	.057001	.056938	.045250	.033954
4.0	32	6.7412	6.6650	.057741	.058588	.045720	.033963
5.0	38	7.9490	7.8504	.058610	.060046	.046189	.034096
6.0	44	9.1514	9.0290	.059478	.061300	.046638	.034288
7.0	50	10.350	10.203	.060304	.062378	.047063	.034508
8.0	56	11.545	11.373	.061074	.063312	.047462	.034741
9.0	62	12.739	12.541	.061786	.064129	.047837	.034976
10	68	13.930	13.706	.062443	.064851	.048188	.035210

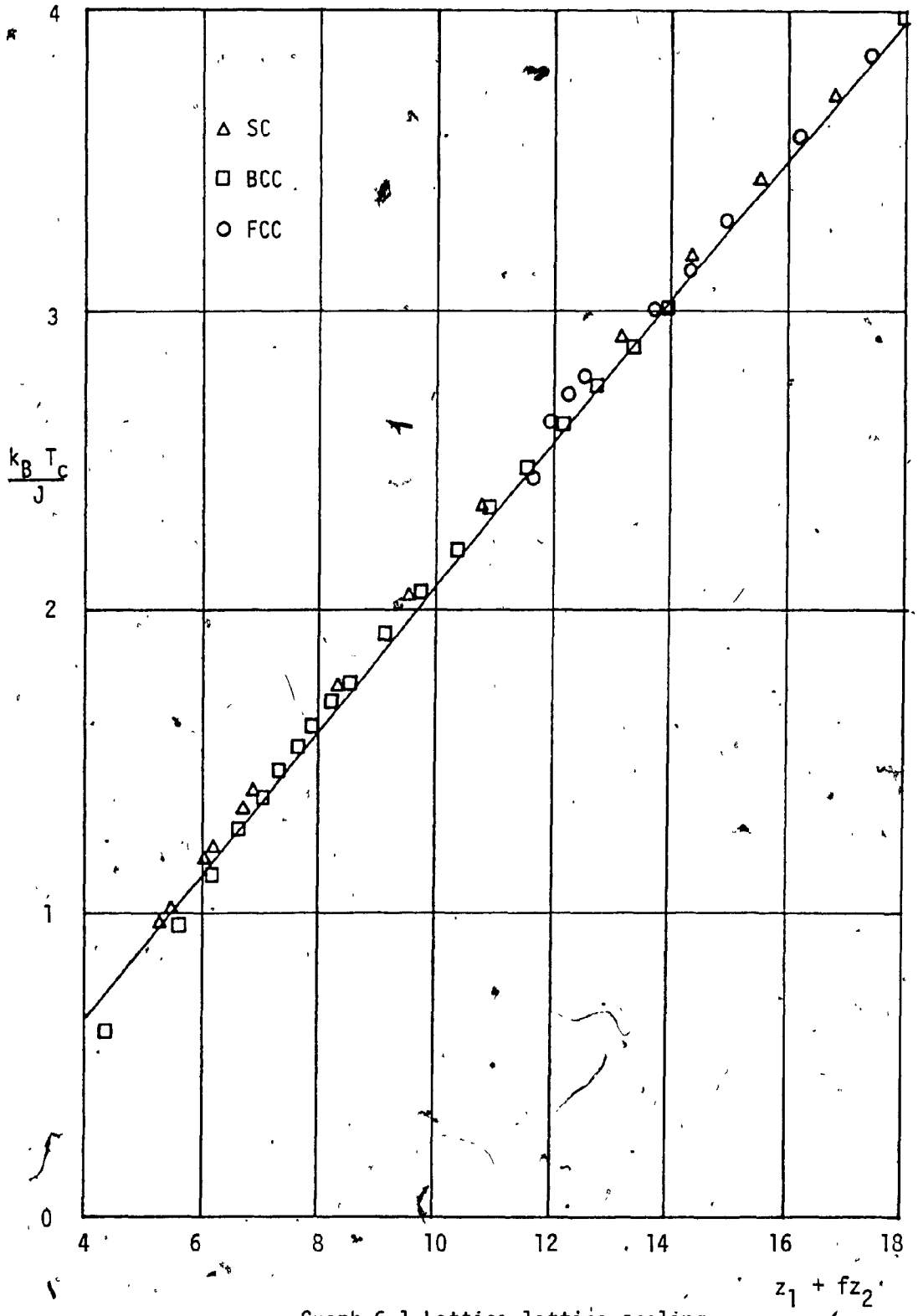
15	98	19.869	19.510	.065076	.067508	.049658	.036288
20	128	25.788	25.289	.066958	.069249	.050763	.037191
30	188	37.590	36.807	.069511	.071481	.052420	.038591
100	608	119.7	116.9	.075740	.076686	.057038	.042894
300	1808	353.2	344.35	.079420	.079812	.060225	.046064
400	2408	469.7	457.9	.080105	.080410	.060858	.046708
1000	6008	1168	1138	.081774	.081907	.062452	.048374
3000	18008	3497	3401	.083253	.083301	.064006	.049990
10000	60008	11760	11236	.084357	.084372	.065193	.051255
30000	180008	34480	30303	.084842	.084847	.065722	.051820

Table 6-3

FCC lattice

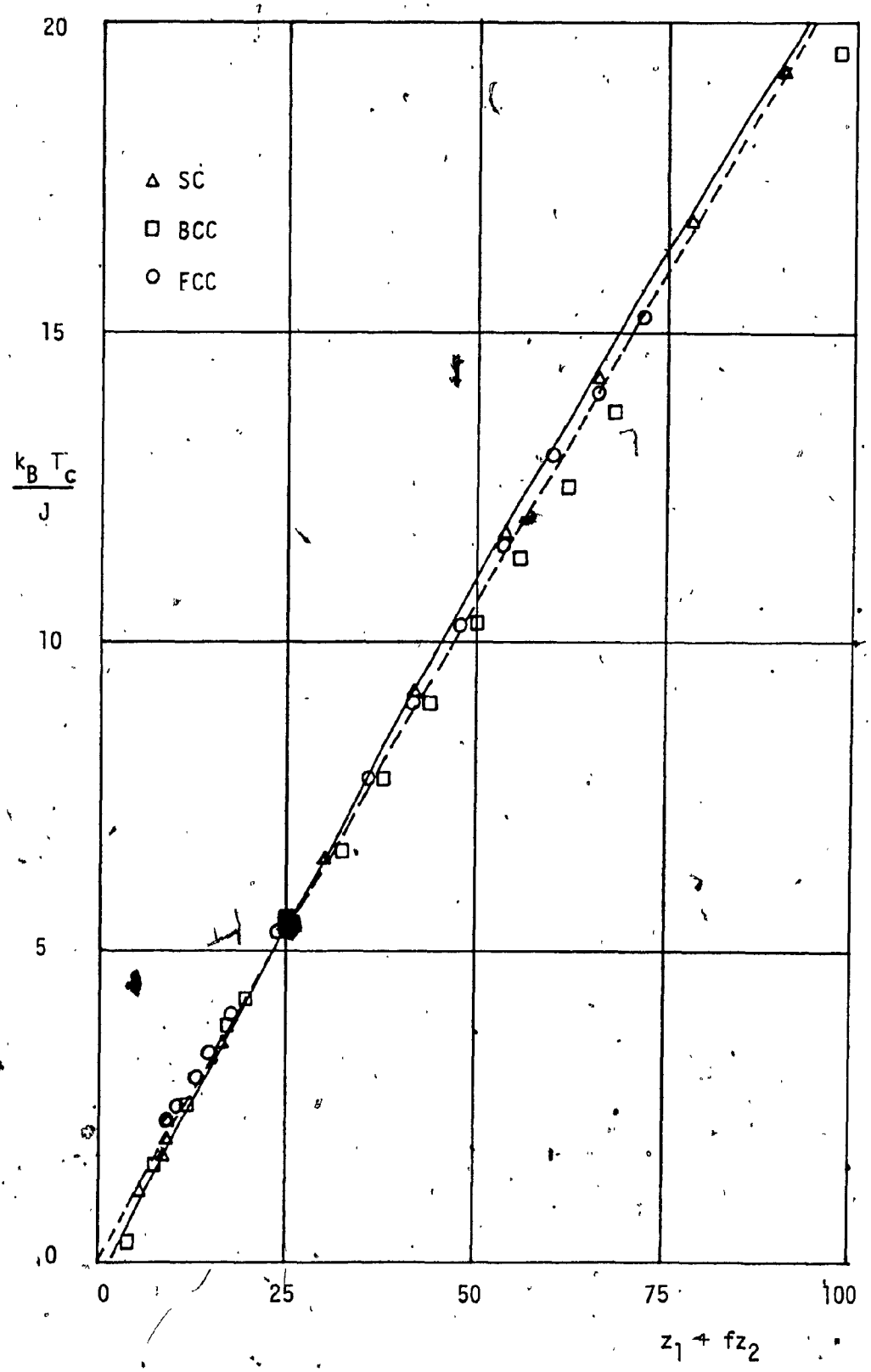
		A=1	A'=1				
f	z_1+fz_2	$1/\beta_c J$	$1/\beta_c J$	T_2	$T_2(\bar{p}_{11},\bar{p}_{22})$	$\bar{p}_{11}$	$\bar{p}_{22}$
-0.06	11.64	2.4339	2.4055	.066306	.066648	.048124	.030484
-0.05	11.7	2.4502	2.4222	.065918	.066199	.047960	.030368
-0.04	11.76	2.4665	2.4388	.065537	.065759	.047799	.030254
-0.03	11.82	2.4827	2.4554	.065163	.065327	.047640	.030142
-0.02	11.88	2.4989	2.4719	.064796	.064903	.047484	.030032
-0.01	11.94	2.5150	2.4884	.064434	.064487	.047330	.029924
-10^{-9}	12	2.5311	2.5048	.064080	.064080	.047178	.029818
10^{-9}	12	2.5311	2.5048	.064080	.064080	.047178	.029818
0.01	12.06	2.5471	2.5212	.063731	.063679	.047028	.029714
0.02	12.12	2.5632	2.5375	.063389	.063287	.046880	.029611
0.03	12.18	2.5791	2.5538	.063052	.062901	.046735	.029511
0.04	12.24	2.5950	2.5700	.062721	.062523	.046591	.029412
0.05	12.30	2.6110	2.5861	.062396	.062152	.046449	.029315
0.06	12.36	2.6268	2.6023	.062077	.061787	.046310	.020219
0.07	12.42	2.6426	2.6183	.061763	.061430	.046172	.029125
0.08	12.48	2.6584	2.6343	.061454	.061079	.046036	.029033
0.09	12.54	2.6742	2.6503	.061151	.060734	.045901	.028942
0.1	12.6	2.6899	2.6662	.060853	.060396	.045769	.028853
0.2	13.2	2.8450	2.8231	.058130	.057334	.044534	.028035
0.3	13.8	2.9968	2.9762	.055819	.054777	.043441	.027337

0.4	14.4	3.1459	3.1259	.053848	.052636	.042465	.026736
0.5	15	3.2729	3.2729	.052161	.050838	.041588	.026216
0.6	15.6	3.4174	3.4174	.050712	.049325	.040793	.025763
0.7	16.2	3.5793	3.5597	.049464	.048052	.040069	.025368
0.8	16.8	3.7200	3.7002	.048387	.046980	.039407	.025022
0.9	17.4	3.8593	3.8391	.047457	.046077	.038798	.024718
1.0	18	3.9972	3.9765	.046653	.045320	.038235	.024451
2.0	24	5.3286	5.2991	.042798	.042334	.034298	.023026
3.0	30	6.6131	6.5708	.042383	.042781	.032004	.022711
4.0	36	7.8749	7.8172	.043080	.044111	.030475	.022823
5.0	42	9.1227	9.0477	.044153	.045623	.029371	.023120
6.0	48	10.361	10.267	.045332	.047100	.028532	.023500
7.0	54	11.592	11.478	.046508	.048477	.027868	.023916
8.0	60	12.818	12.683	.047637	.049739	.027327	.024344
9.0	66	14.039	13.882	.048703	.050889	.026877	.024769
10	72	15.256	15.077	.049700	.051939	.026496	.025185
15	102	21.305	21.007	.053782	.056027	.025207	.027061
20	132	27.313	26.889	.056752	.058858	.024451	.028596
30	192	39.259	38.569	.060808	.062607	.023581	.030932
100	612	121.2	119.3	.070679	.071521	.021969	.037888
300	1812	356.4	347.8	.076421	.076762	.021260	.042862
400	2412	473.3	461.7	.077479	.077743	.021143	.043860
1000	6012	1174	1144	.080043	.080157	.020882	.046424
3000	18012	3497	3401	.082297	.082337	.020678	.048886
10000	60012	11900	11236	.083965	.083978	.020538	.050798

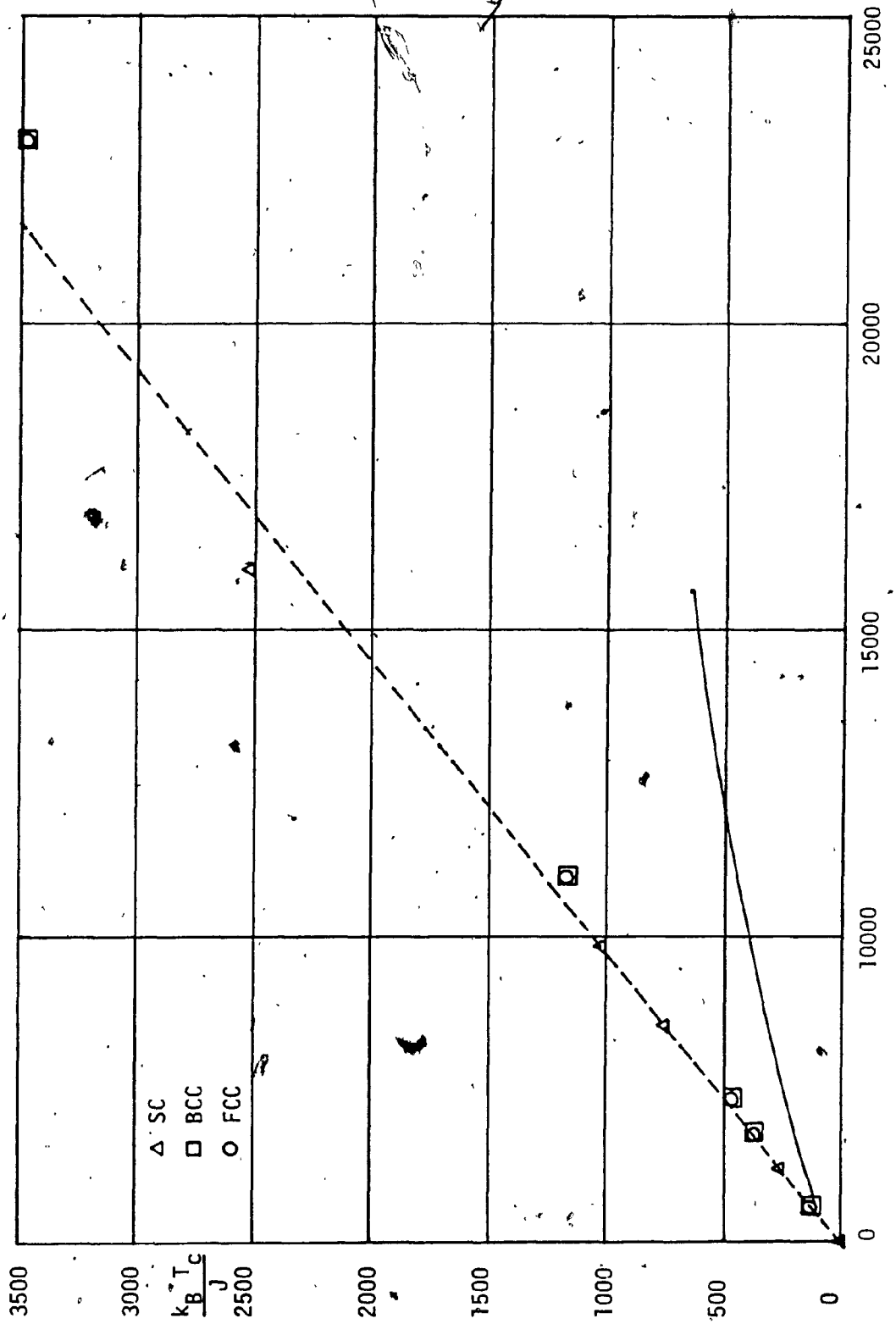


Graph 6-1 Lattice-lattice scaling

Graph 6-2 Lattice-lattice scaling



Graph 6-3 Lattice-lattice scaling



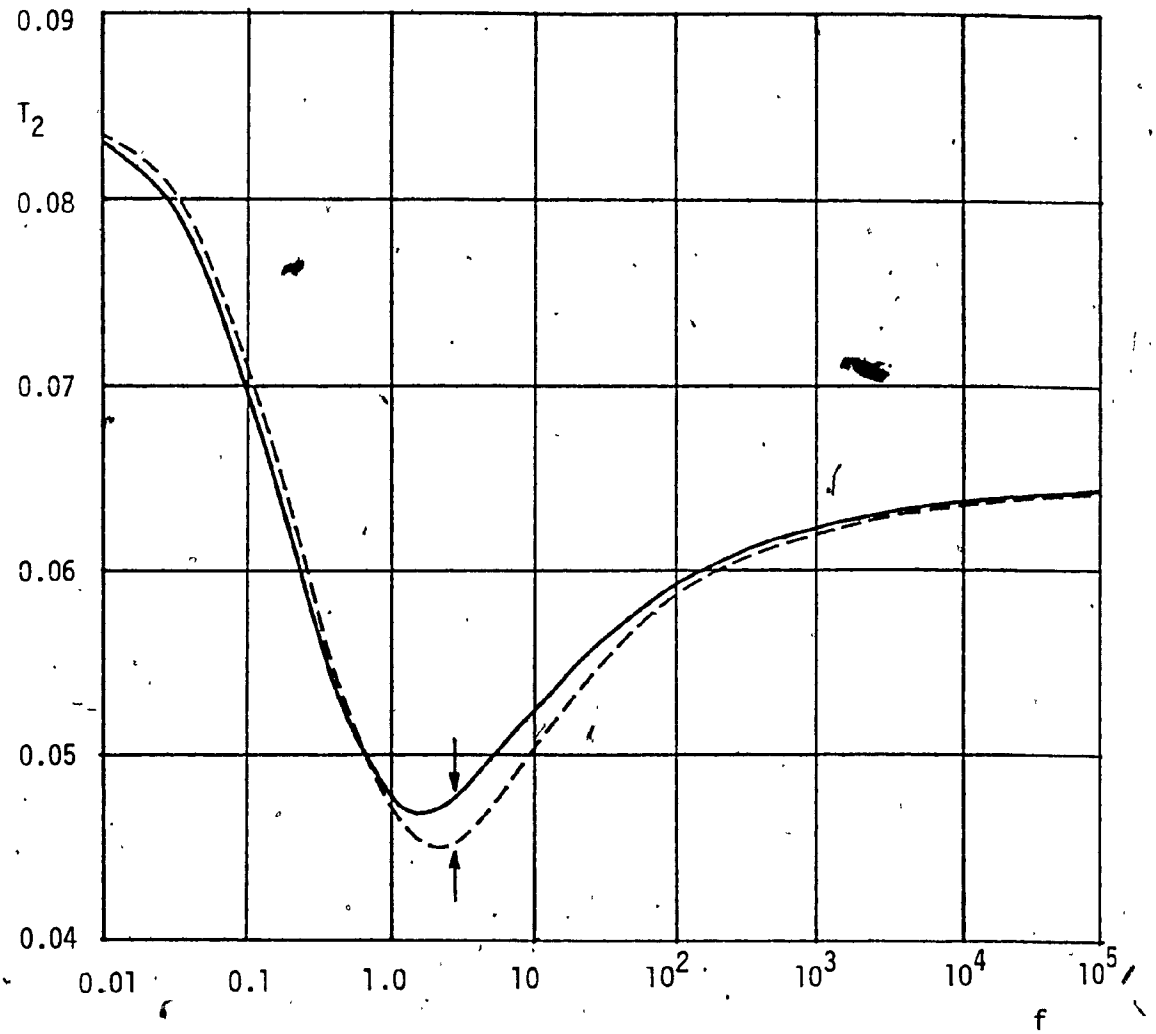
6-1-2 Behaviour of the T_2's

We now compare the $T_2(\bar{p}_{11},\bar{p}_{22})$ using (95) (after $\bar{p}_{11}$ and $\bar{p}_{22}$ chosen were known from (97) and (98)) with the T_2 obtained directly from (82) and (74); the numerical values of these functions are in Tables 6-1, 6-2 and 6-3.

The difference between the two T_2's vanishes either when $f \to 0$ or when $f \to \infty$ as can be expected directly from the definitions.

The T_2's are plotted as functions of f in graph 6-4. The largest discrepancies are indicated by arrows on the graphs and are given in Table 6-4, they are of the order of a few percent. One can then expect that our critical temperatures differ, by the order of a few percent as well, when compared to series results.

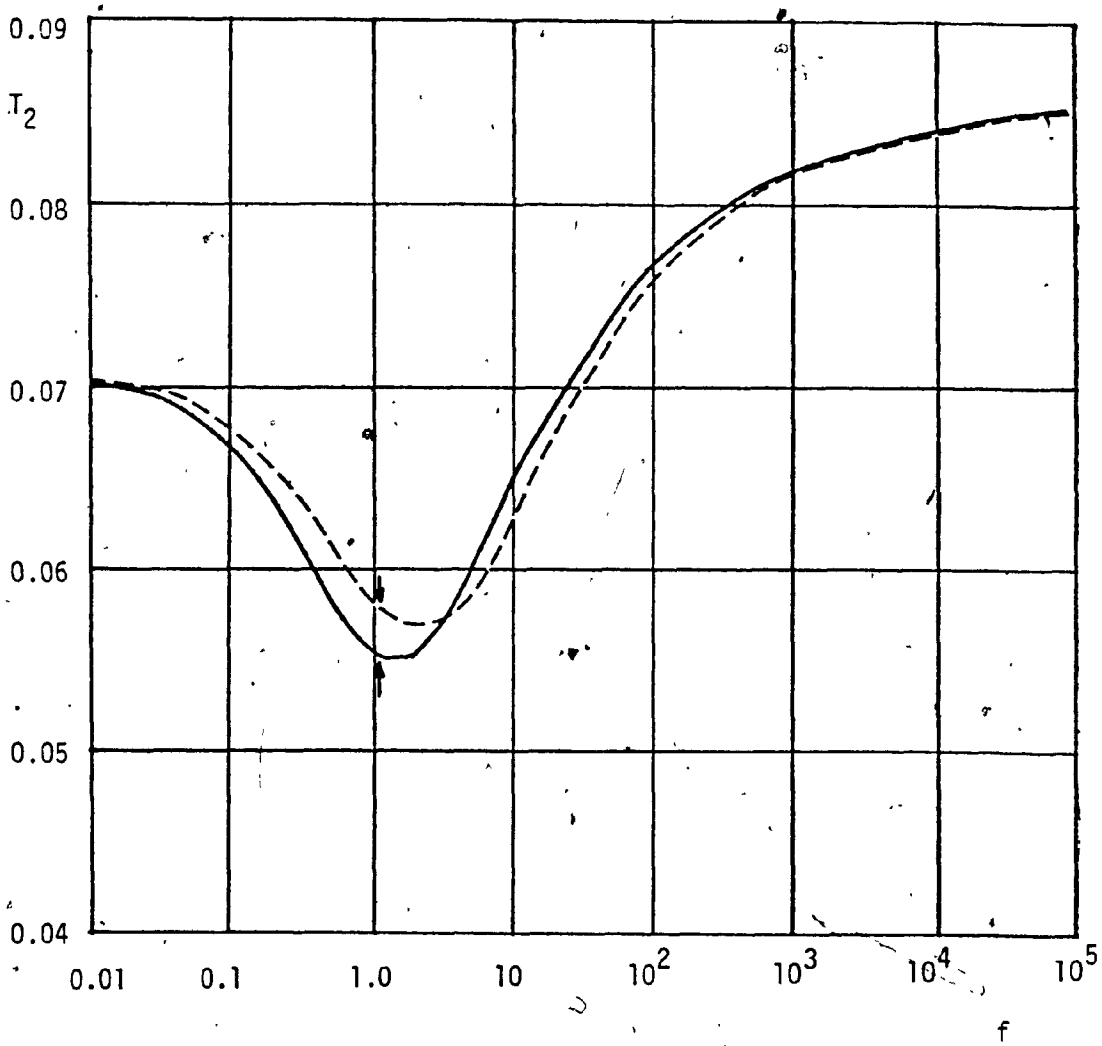
Graph 6-4 (a) T_2's for SC lattice



T_2 ------

$T_2(\bar{p}_{11}, \bar{p}_{22})$ ——————

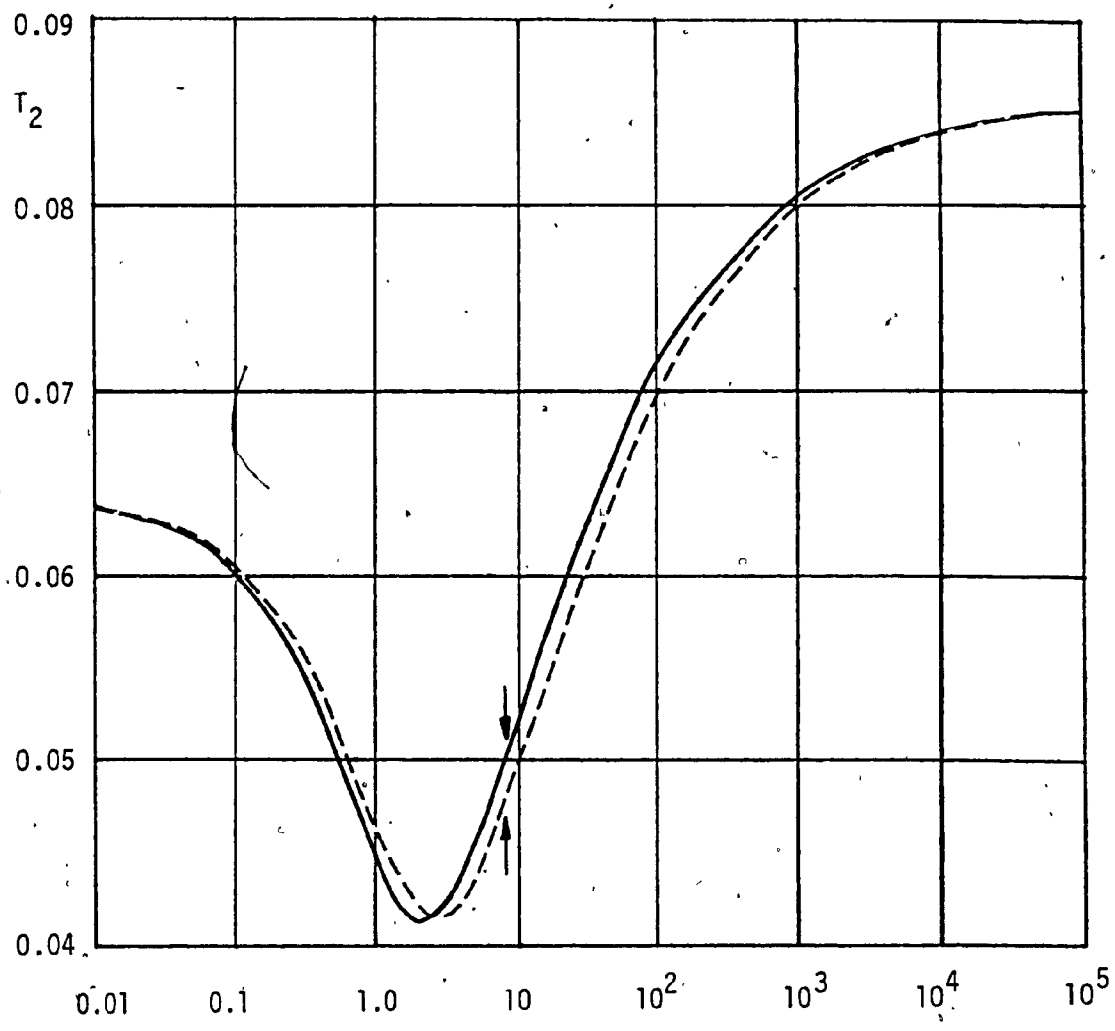
Graph 6-4 (b) T_2's for BCC lattice



T_2 ——— —

$T_2(\bar{p}_{11}, \bar{p}_{22})$ ———

Graph 6-4 (c) T_2's for FCC lattice



T_2 ----------

$T_2(\bar{p}_{11}, \bar{p}_{22})$ ——————

Table 6-4

Greatest discrepancies between T_2 and $T_2(\bar{p}_{11}, \bar{p}_{22})$

lattice	discrepancy
SC	6 %
BCC	5.5 %
FCC	4.3 %

6-1-3 Lattice-lattice scaling

A remarkable feature of the graphs 6-1, 6-2 and 6-3 is that the critical temperatures for all three cubic lattices lie on the same curve within the error one can expect from the partial T_2's assumption.

We tried to fit a first degree or a second degree polynomial, by least squares, to the whole data of Tables 6-1, 6-2 and 6-3; neither of those fitted the data , to a few percent, for the whole range. The best fit is, in fact a second degree polynomial for the first part of the data; i.e. roughly for $z_1 + fz_2$ not exeeding a few tens; and a first degree polynomial for the rest of the range.

Using:

$$k_B T_c(f)/ J = Y$$

and (160)

$$z_1 + fz_2 = X,$$

the linear relation, obtained by least squares fitting, is:

$$Y = m X + b$$

where:

$$m = 0.21265,$$

and (161)

$$b = 0.04846$$

that is the straight line on graphs 6-2 and 6-3.

The quadratic relation, also fitted by least squares, is, with definitions (160):

$$X = a_0 + a_1 Y + a_2 Y^2$$

where:

$$a_0 = 1.28914$$

$$a_1 = 4.10293 \qquad (162)$$

$$a_2 = 0.02345,$$

that is the curve appearing on graphs 6-1 and 6-2.

We therefore confirm the "slight curvature" cited by Dalton and Wood (1969). We also find that the curvature seems to vanish as the value of f (or $z_1 + fz_2$) increases, suggesting an asymptotic behaviour.

6-1-4 Negative values of f

The constant a_0 in (162) has a particularly simple interpretation since it is the value of $z_1 + fz_2$ for which $k_B T_c / J$ vanishes. The values of f for which the system has a vanishing critical temperature can then be evaluated for the cubic lattices; they are given in Table 6-5. They are extrapolations and as such are not reliable; BCC and FCC values are out of the range estimated by Dalton and Wood (1969).

The negative values of f signify that there are competing interactions between first and second neighbours but the system remains ferromagnetic; for values of f lower than those of Table 6-5 the system has no ferromagnetic transition.

Table 6-5

lower limit of f

lattice	present work	Dalton & wood
SC	-0.39	$-0.4 \leq f \leq -0.7$
BCC	-1.12	$-0.8 \leq f \leq -0.6$
FCC	-1.79	$-1.0 \leq f \leq -0.7$

6 - 2 Comparison with available data

6-2-1 Series results

Table 6-6 contains the ratios of the critical temperatures for the first and second neighbours system to the critical temperature of the first neighbour system $(T_c(f)/T_c(0))$, calculated for the three cubic lattices using Tables 6-1, 6-2 and 6-3. The ratios given by Dalton and Wood (1969) also appear in Table 6-6 for comparison purposes. Dalton and Wood (1969) proposed:

$$T_c(f)/T_c(0) = 1 + m\,f \qquad (163)$$

The last four lines in Table 6-6 give the parameters of (163) obtained by the least squares fitting of a straight line to the data; the third of these lines is the difference, in percentage, between the Dalton and Wood slopes and ours; the last line is the coefficient of correlation. The Dalton and Wood slopes are not the slopes appearing in their paper; we used their data with our program (REGRE in Appendix L) since we do not know how they calculated their slopes. The straight lines on graphs 6-5, 6-6 and 6-7 are the Dalton and and Wood ones resulting from the above calculation.

The difference between the series calculation and our method decreases as the number of neighbouring sites taken into account increases, as was pointed out by Dalton and Wood (1969). Our FCC results confirm that tendency, as can be seen directly from Table 6-6 or from the graphs 6-5, 6-6 and 6-7.

We also remark that the critical condition A = 1 leads to critical temperatures closer to those obtained by series than does A'= 1; this was already pointed out in other contexts by Girvin (1978) and by Frank, Cheung and Mouritsen (1982).

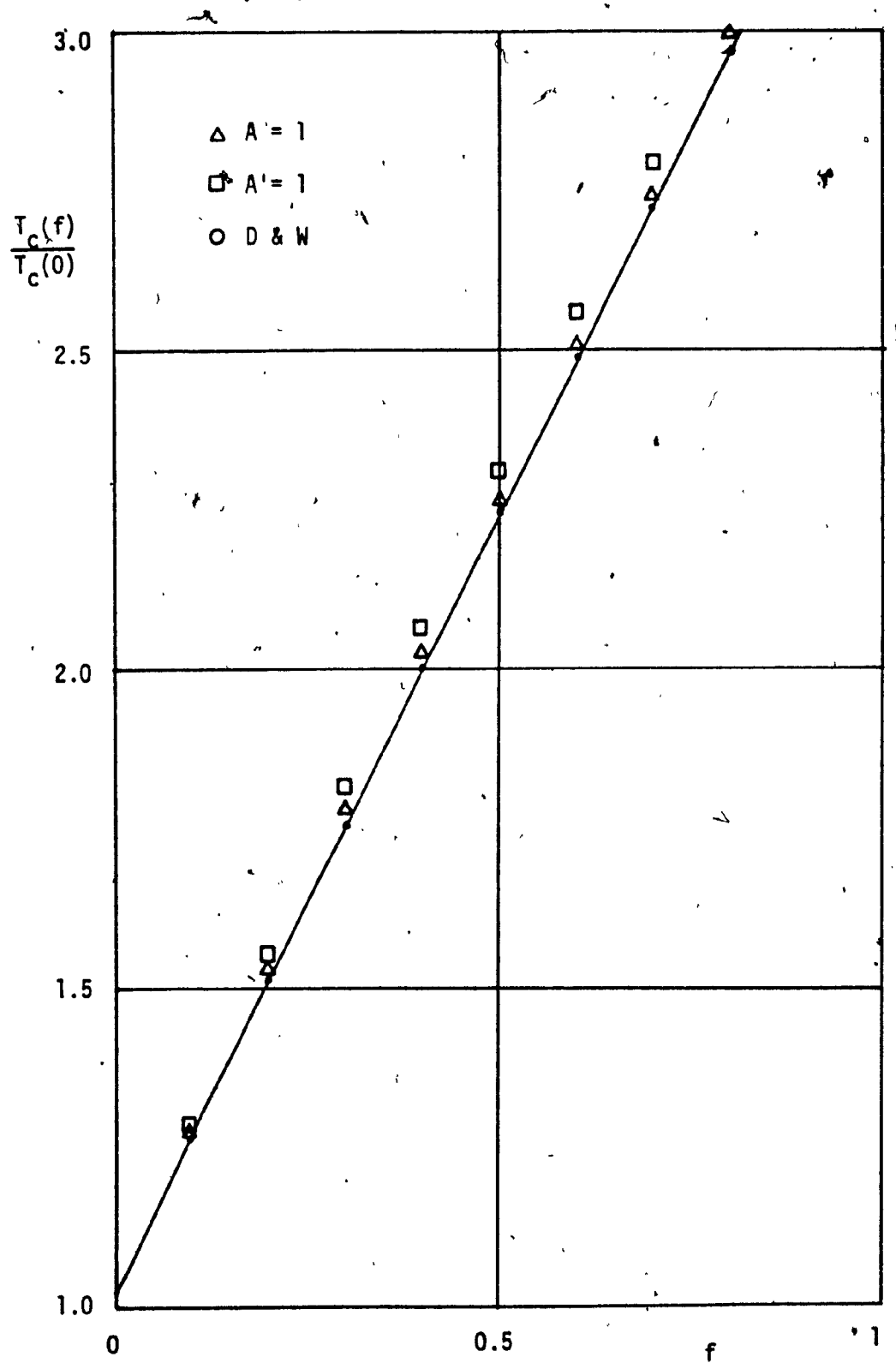
Table 6-6

ratios

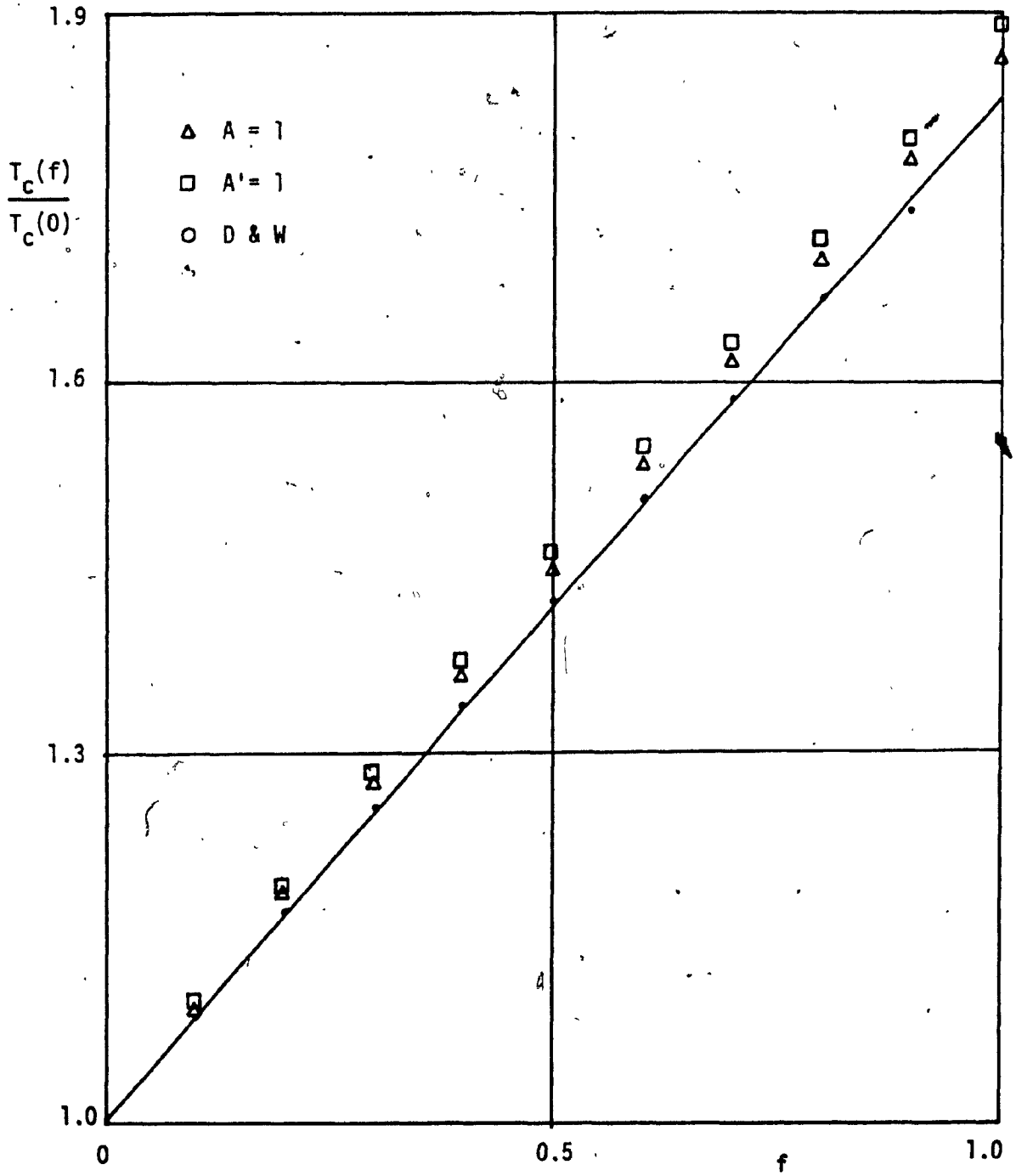
$$T_c(f)/T_c(0) = \beta_c(0)/\beta_c(f)$$

	SC			BCC			FCC		
f	D & W	A = 1	A'= 1	D & W	A = 1	A'= 1	D & W	A = 1	A'= 1
0.1	1.260	1.271	1.287	1.085	1.094	1.098	1.061	1.063	1.064
0.2	1.513	1.531	1.556	1.170	1.185	1.192	1.119	1.124	1.127
0.3	1.761	1.787	1.816	1.255	1.275	1.284	1.182	1.184	1.188
0.4	2.002	2.026	2.067	1.239	1.362	1.373	1.240	1.243	1.248
0.5	2.298	2.267	2.315	1.422	1.448	1.460	1.299	1.301	1.307
0.6	2.489	2.505	2.558	1.505	1.532	1.546	1.357	1.358	1.364
0.7	2.728	2.741	2.799	1.587	1.616	1.630	1.413	1.414	1.421
0.8	2.965	2.974	3.038	1.668	1.698	1.714	1.470	1.470	1.477
0.9	3.200	3.207	3.276	1.749	1.779	1.796	1.526	1.525	1.533
1.0	3.435	3.438	3.510	1.829	1.860	1.877	1.582	1.579	1.587
slope	2.428	2.423	2.492	0.8295	0.8574	0.8735	0.582	0.578	0.586
		0.2	2.5		3.2	5		0.7	0.7
intercept	1.027	1.038	1.047	1.004	1.012	1.015	1.004	1.008	1.009
correlation	.99964	.99971	.99962	.99994	.99972	.99961	.99988	.99976	.99968

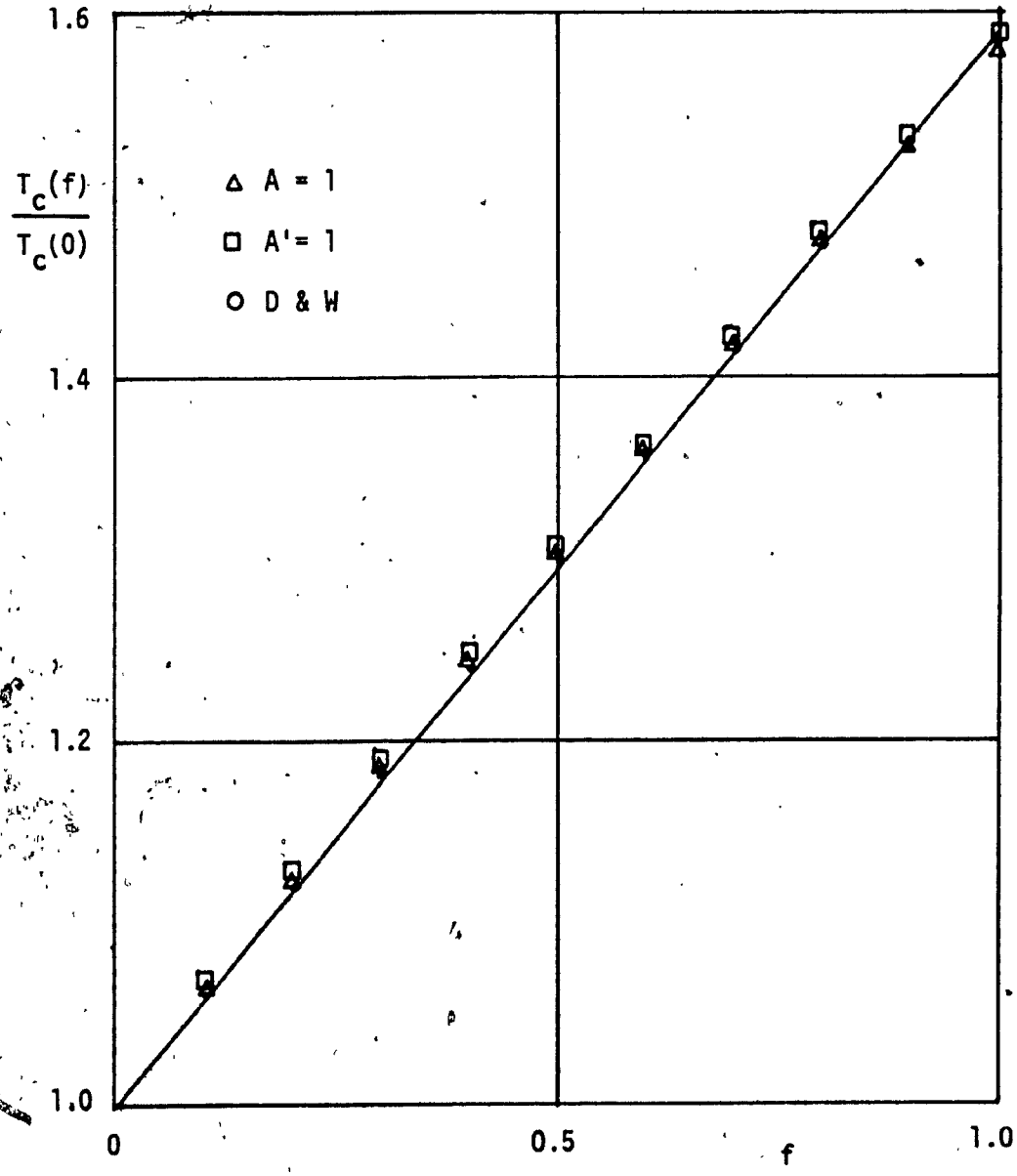
Graph 6-5 Ratios for SC lattice



Graph 6-6 Ratios for BCC lattice



Graph 6-7 Ratios for FCC lattice



6-2-2 Hypercubic lattices

Nath and Frank (1982) and also Nath (1984) calculated $k_B T_c/J$ for hypercubic lattices of dimensionality 4 to 30, using the i-δ relations, for first neighbours only. Their results are in Table 6-6; they are rewritten according to our definitions of the variables. Taking the number of first neighbours Z as an "equivalent number of neighbours", we can compare their results with ours. Their slope, given in Table 6-7, is larger than our main slope (161) by some 20 %; that discrepancy cannot be attributed to the assumptions made in the theory; it might be a clear effect of the second neighbours on T_c.

Table 6-[illegible]

Hypercubic lattices

Z	$1/\beta_c J$
8	1.687
10	2.210
12	2.722
14	3.229
16	3.733
18	4.236
20	4.738
30	7.243
40	9.745
50	12.246
60	14.747
slope	0.251
intercept	-0.289
correlation	.9999958

6 - 3 Concluding remarks

We calculated the critical temperature for the Ising ferromagnet, including second neighbours, using a relatively simple method compared to series expansions. That simplicity allowed us to go far beyond the values of f in current literature, e.g. Tables 6-1, 6-2 and 6-3 compared to Table 6-6.

In the development of the method we derived formulas, for the first time, to obtain the points and weighting factors of the Chadi and Cohen scheme.

The present theory can certainly be applied to two -dimensional lattices with similar success for the same computer time. It would also be interesting to see, in higher dimensions, how the discrepancy between our slope (161) and that of Nath and Frank (1984) or Nath (1982) behaves.

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Appendix A: Evaluation of $\mathrm{Tr}\{\exp(-\bar{\beta}O_i S_i)\}$

Starting with (52) in the denominator of (51):

$$\mathrm{Tr}\{\exp(-\bar{\beta}O_i S_i)\}$$

$$= \mathrm{Tr}\{\exp[(-\bar{\beta}S_i(J_1 \sum_{j=1}^{\text{st}} S_j + J_2 \sum_{k=2}^{\text{nd}} S_k)]\} \qquad (A\text{-}1)$$

$$= \mathrm{Tr}\{\exp(-J_1\bar{\beta}S_i S_{j_1}) \exp(-J_1\bar{\beta}S_i S_{j_2}) \text{ ---}$$

$$\text{--- } \exp(-J_1\bar{\beta}S_i S_{j_{z_1}})$$

$$\times \exp(-J_2\bar{\beta}S_i S_{k_1}) \text{ ---- } \exp(-J_2\bar{\beta}S_i S_{k_{z_2}})\} \qquad (A\text{-}2)$$

noticing that

$$\exp x = \cosh x + \sinh x = \cosh x\,(1 + \tanh x) \qquad (A\text{-}3)$$

$$\exp(-J\bar{\beta}\, S_i S_\ell) = \cosh(J\bar{\beta}\, S_i S_\ell)[1 - \tanh J\bar{\beta}S_i S_\ell] \qquad (A\text{-}4)$$

with $S_i S_\ell = \pm 1/4$ and since cosh is an even function

$$= \cosh(\bar{\beta}J/4)[1 - \tanh \bar{\beta}J\, S_i S_\ell] \qquad (A\text{-}5)$$

one has

$$\mathrm{Tr}\{\exp(-\bar{\beta}\, O_i\, S_i)\}$$

$$= \mathrm{Tr}\Big\{\prod_{j=1}^{st} \cosh(\bar{\beta} J_1/4)(1-\tanh \bar{\beta} J_1 S_i S_j)$$

$$\times \prod_{k=2}^{nd} \cosh(\bar{\beta} J_2/4)(1-\tanh \bar{\beta} J_2 S_i S_k)\Big\} \qquad \text{(A-6)}$$

or:

$$\mathrm{Tr}\{\exp(-\bar{\beta}\, O_i\, S_i)\} = \cosh^{z_1}(\bar{\beta} J_1/4)\cosh^{z_2}(\bar{\beta} J_2/4) \qquad \text{(A-7)}$$

which is equation (54).

Appendix B: Evaluation of

$$(\partial^{2n}/\partial\bar{\beta}^{2n})[\cosh^{z_1}(\bar{\beta}J_1/4)\cosh^{z_2}(\bar{\beta}J_2/4)] \tag{B-1}$$

Using $\cosh^z x = (1/2^z)(e^x + e^{-x})^z$ (B-2)

one has

$$\cosh^{z_1}(\bar{\beta}J_1/4)\cosh^{z_2}(\bar{\beta}J_2/4)$$

$$= (1/2^{z_1+z_2})[\exp(\bar{\beta}J_1/4) + \exp(-\bar{\beta}J_1/4)]^{z_1}$$

$$x[\exp(\bar{\beta}J_2/4) + \exp(-\bar{\beta}J_2/4)]^{z_1} \tag{B-3}$$

$$= 1/2^{z_1+z_2} \sum_{\lambda=0}^{z_1} C_\lambda^{z_1} \exp(\bar{\beta}J_1/4)^{z_1-\lambda} \exp(\bar{\beta}J_1/4)^{\lambda}$$

$$x \sum_{\mu=0}^{2} C_\mu^{z_1} \exp(\bar{\beta}J_2/4)^{z_2-\mu} \exp(-\bar{\beta}J_2/4)^{\mu} \tag{B-4}$$

where we used

$$(a+b)^n = \sum_{p=0}^{n} C_p^n \, a^{n-p} \, b^p \quad \text{and} \quad C_p^n = n!/p!(n-p)!$$

than

$$(\partial^{2n}/\partial\bar{\beta}^{2n})[\cosh^{z_1}(\bar{\beta}J_1/4)\cosh^{z_1}(\bar{\beta}J_2/4)]$$

$$=(\partial^{2n}/\partial\bar{\beta}^{2n})[1/2^{z_1+z_2} \sum_{\lambda=0}^{z_1} C_\lambda^{z_1} \exp(z_1-2\lambda)\bar{\beta}J_1/4$$

$$x \sum_{\mu=0}^{z_2} \exp(z_2-2\mu)\bar{\beta}J_2/4 \tag{B-5}$$

A4

$$= (1/2^{z_1+z_2} \sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\mu^{z_2} [(z_1-2\lambda)J_1/4 + (z_2-2\mu)J_2/4]^{2n}$$

$$\times \exp \beta[(z_1 - 2\mu)J_1/4 + (z_2 - 2\mu)J_2/4] \qquad \text{(B-6)}$$

which is equation (57)

Appendix C: from (61) to (62)

$$T_{2n}= \quad 2^{2n}\Bigg[\sum_{\lambda=0}^{z_1}\sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\mu^{z_2} [D(\lambda,\mu)]^{2n}\left[(1-q_{11})/(1+q_{11})\right]^{-\lambda+z_1/2} \times \left[(1-q_{22})/(1+q_{22})\right]^{-\mu+z_2/2}\Bigg]$$

$$/\Bigg[(z_1J_1+z_2J_2)^{2n}\sum_{\delta=0}^{z_1}\sum_{\varepsilon=0}^{z_2} C_\delta^{z_1} C_\varepsilon^{z_2}\left[(1-q_{11})/(1+q_{11})\right]^{-\delta+z_1/2} \times \left[(1-q_{22})/(1+q_{22})\right]^{-\varepsilon+z_2/2}\Bigg] \qquad (61)$$

the summations in the denominator can be written:

$$\sum_{\delta=0}^{z_1} \left((1-q_{11})/(1+q_{11})\right)^{z_1/2} C_\delta^{z_1}\left((1+q_{11})/(1-q_{11})\right)^{\delta} \times \sum_{\varepsilon=0}^{z_1} C_\varepsilon^{z_2} \left((1=q_{22})/(1+q_{22})\right)^{z_2/2} \left((1+q_{22})/(1-q_{22})\right)^{\varepsilon} \qquad (C\text{-}1)$$

$$= \left((1-q_{11})/(1+q_{11})\right)^{z_1/2} \left((1-q_{22})/(1+q_{22})\right)^{z_2/2} \times \sum_{\delta=0}^{z_1} C_\delta^{z_1}\left((1+q_{11})/(1-q_{11})\right)^{\delta} \times \sum_{\varepsilon=0}^{z_1} C_\varepsilon^{z_1}\left((1+q_{22})/(1-q_{22})\right)^{\varepsilon} \qquad (C\text{-}2)$$

Multiplying the δ summation by $1^{z_1-\delta}$ and the ϵ summation by $1^{z_1-\epsilon}$ one has:

$$((1-q_{11})/(1+q_{11}))^{z_1/2} \quad ((1-q_{22})/(1+q_{22})^{z_2/2}$$

$$\times [1+((1+q_{11})/(1-q_{11}))]^{z_1} \; [1+((1+q_{22})/(1-q_{22}))]^{z_2} \qquad \text{(C-3)}$$

$$= 2^{z_1+z_2} ((1-q_{11})/(1+q_{11}))^{z_1/2} \quad ((1-q_{22})/(1+q_{22}))^{z_2/2}$$

$$/[(1-q_{11})^{z_1} (1-q_{22})^{z_2}] \qquad \text{(C-4)}$$

$$= 2^{z_1+z_2} (1-q_{11})^{-z_1/2} (1+q_{11})^{-z_1/2} (1-q_{22})^{-z_2/2} (1+q_{22})^{-z_2/2}. \qquad \text{(C-5)}$$

Using (C-5) in the summation of the denominator of (61):

$$T_{2n} = 2^{2n-z_1-z_2} (z_1J_1+z_2J_2)^{-2n} \sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\mu^{z_2}$$

$$\times [D(\lambda,\mu)]^{2n} \quad (1-q_{11})^{-\lambda+z_1/2} (1+q_{11})^{\lambda-z_1/2} (1-q_{22})^{-\mu+z_2/2}$$

$$\times (1+q_{22})^{\mu-z_2/2} (1+q_{11})^{z_1/2} (1+q_{11})^{z_1/2}$$

$$\times (1-q_{22})^{z_1/2} (1+q_{22})^{z_2/2} \qquad \text{(C-6)}$$

$$= 2^{2n-z_1-z_2} (z_1J_1+z_2J_2)^{-2n} \sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\mu^{z_2} [D(\lambda,\mu)]^{2n}$$

$$\times (1-q_{11})^{z_1-\lambda} (1+q_{11})^{\lambda} (1-q_{22})^{z_2-\mu} (1+q_{22})^{\mu} \qquad \text{(C-7)}$$

or finally:

$$T_{2n} = 2^{-z_1-z_2} \sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\mu^{z_2} [2D(\lambda,\mu)/(z_1J_1+z_2J_2)]^{2n}$$

$$\times (1-q_{11})^{z_\lambda-\lambda} (1+q_{11})^{\lambda} (1-q_{22})^{z_2-\mu} (1+q_{22})^{\mu} \qquad (62)$$

which is the result sought.

Appendix D: 64 in (21)

Equation (21) is, introducing $J(0)/J(0) = 1$:

$$\langle \tanh^2 (\beta_c J(0) O_1 / 2J(0)) \rangle / 2 = \langle (O_i / J(0)) \tanh (\beta_c J(0) O_1 / 2J(0)) \rangle . \tag{D-1}$$

then, using (64) directly, (D-1) becomes:

$$2^{-(z_1+z_2+1)} \sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\mu^{z_2} (1-q_{11})^{z_1-\lambda} (1+q_{11})^{\lambda} (1-q_{22})^{z_2-\mu} (1+q_{22})^{\mu}$$

$$\times \tanh^2 [\beta_c J(0) D(\lambda,\mu) / (z_1 J_1 + z_2 J_2)]$$

$$= 2^{-(z_1+z_2)} \sum_{\varepsilon=0} \sum_{\delta=0} (1-q_{11})^{z_1-\varepsilon} (1+q_{11})^{\varepsilon} (1-q_{22})^{z_2-\delta} (1+q_{22})^{\delta}$$

$$\times 2D(\lambda\ \mu)(z_1 J_1 + z_2 J_2)$$

$$\times \tanh [\beta_c J(0)\ D(\lambda,\mu) / (z_1\ J_1 + z_2\ J_2] \tag{D-2}$$

Since $J(0) = z_1 J_1 + z_2 J_2$ (see e.g., (14 and (1)),

with rearranging:

$$\sum_{\lambda=0} \sum_{\mu=0} C_\lambda^{z_1} C_\mu^{z_2} (1-q_{11})^{z_1-\lambda} (1+q_{11})^{\lambda} (1-q_{22})^{z_2-\mu} (1+q_{22})^{\mu}$$

$$\times \tanh \beta_c D(\lambda,\mu) [(1/2) \tanh (\beta_c D(\lambda,\mu)) - 2D(\lambda,\mu)/z_1 J_1 + z_2 J_2)] = 0$$

(D-3)

Or, substituting $D(\lambda,\mu)$ from (59):

$$\sum_{\lambda=0}^{z_1}\sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\mu^{z_2} (1-q_{11})^{z_1-\lambda}(1+q_{11})^{\lambda}(1-q_{22})^{z_1-\mu}(1+q_{22})^{\mu}$$

$$\times \tanh\left(\beta_c(J/4)[(z_1-2\lambda) + (z_2-2\mu)\, f\right])$$

$$\times \quad (1/2)\, \tanh\left(\beta_c(J/4)\, [(z_1-2\lambda) + (z_2-2\mu)f]\right)$$

$$- [z_1-2\lambda + (z_2-2\mu)f]/2\,(z_1+fz_2) \quad = 0 \qquad \text{(D-4)}$$

noticing that the 1/2 in the double square bracket can be taken out of the summation and then dropped, we have equation (65).

Appendix E: (64) in (22)

Introducing $J(0)/J(0) = 1$ and rearranging, equation (22) is:

$$\langle (\sigma_i/J(0)) \tanh [\beta_c J(0)\, \sigma_i/2J(0)] \rangle = 2\langle \sigma_i^2 \rangle / J^2(0). \qquad \text{(E-1)}$$

Using (64), (E-1) becomes

$$2^{-(z_1+z_2)} \sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} C_\lambda^{z_1} C_\mu^{z_2} (1-q)^{z_1-\lambda} (1+q_{11})^{\lambda} (1-q_{22})^{z_2-\mu} (1+q_{22})^{\mu}$$

$$\times\, 2D(\lambda,\mu)/(z_1 J_1 + z_2 J_2)$$

$$\times \tanh [\beta_c J(0)\, D(\lambda,\mu)/(z_1 J_1 + z_2 J_2)]$$

$$= 2 \times 2^{z_1+z_2} \sum_{\delta=0}^{z_1} \sum_{\varepsilon=0}^{z_2} C_\delta^{z_1} C_\varepsilon^{z_2} (1-q_{11})^{z_1-\delta} (1+q_{11})^{\delta} (1-q_{22})^{z_2-\varepsilon} (1+q_{22})^{\varepsilon}$$

$$\times\, [2D(\lambda,\mu)/(z_1 J_1 + z_2 J_2)]^2 . \qquad \text{(E-2)}$$

this can be written

$$\sum_{\lambda=0} \sum_{\mu=0} C_\lambda^{z_1} C_\mu^{z_1} (1-q_{11})^{z_1-\lambda} (1+q_{11})^{\lambda} (1-q_{22})^{z_2-\mu} (1+q_{22})^{\mu}$$

$$\times\, 2D(\lambda,\mu)/(z_1 J_1 + z_2 J_2)$$

$$\times \tanh (\beta_c J(0) D(\lambda,\mu)/(z_1 J_1 + z_2 J_2))$$

$$- 4D(\lambda,\mu)/(z_1 J_1 + z_2 J_2)] = 0 \qquad \text{(E-3)}$$

substituting $D(\lambda,\mu)$ from (59), using $J_2 = fJ_1 \equiv fJ$, and (67), one has

$$D(\lambda,\mu)/(z_1J_1 + z_2J_2) = C(\lambda,\mu)/4(z_1 + fz_2) \; ; \qquad \text{(E-4}$$

so that (E-3) becomes, using (66)

$$\sum_{\lambda=0}^{z_1} \sum_{\mu=0}^{z_2} Q(\lambda,\mu)\, C\,(\lambda,\mu)/2(z_1 + fz_2)$$

$$\times \left[\tanh\left(\beta_c\, JC(\lambda,\mu)/4\right) - C(\lambda,\mu)/(z_1 + fz_2)\right] = 0 \qquad \text{(E-5)}$$

Since $2\,(z_1 + fz_2) \neq 0$ it can be removed safely from (E-5) and we have the result (68)

Appendix F: Lattice Green's Functions

We derive here the explicit forms of the lattice Green's functions appearing in (74)

$$F = (1/N) \sum_{\vec{k}} [1-J(\vec{k})/J(0)]^{-1} \qquad (74)$$

where:

$$J(\vec{k}) = \sum_{\ell=1^{st},\ 2^{nd}} J_{i\ell} \exp [i\vec{k}.(\vec{R}_\ell - \vec{R}_i)] , \qquad (13)$$

$$J(0) = J(z_1 + fz_2) \qquad (14)$$

the dot product in the exponential is

$$\vec{k}.(\vec{R}_i - \vec{R}_\ell) = k_x(\vec{R}_\ell - \vec{R}_i)_x + k_y(\vec{R}_\ell - \vec{R}_i)_y + k_z(\vec{R}_\ell - \vec{R}_i)_z . \qquad (F\text{-}1)$$

The numerical values of the Green's functions were obtained as functions of f by the extrapolated Chadi-Cohen (1973) method described in Chapter 3. The f=0 case can be evaluated analytically (Watson 1939) and permits us to evaluate the quality of the approximation.

F - 1: Simple Cubic Lattice

In the simple cubic lattice the first neighbours of site i one easily seem to be (where a is the lattice constant):

$$(\vec{R}_j - \vec{R}_i) = \begin{matrix} (\pm a, 0, 0) \\ (0, \pm a, 0) \\ (0, 0, \pm a) \end{matrix} \qquad \text{(F-2)}$$

and there are $z_1=6$ of them. The second neighbours of site i are given by

$$(\vec{R}_k - \vec{R}_i) = \begin{matrix} (\pm a, \pm a, 0) \\ (\pm a, 0, \pm a) \\ (0, \pm a, \pm a) \end{matrix} \qquad \text{(F-3)}$$

and there are $z_2 = 12$ of them.

For the first neighbours only, using (F-2) in (F-1) together with $J_{i\ell} = J$ and $a = 1$ we get:

$$J \sum_{j=1}^{z_1} \exp\left[i\vec{k}.(\vec{R}_j - \vec{R}_i)\right]$$

$$= [\exp(ik_x) + \exp(-ik_x) + \exp(ik_y) + \exp(-ik_y) + \exp(ik_z) + \exp(-ik_z)] \qquad \text{(F-4)}$$

$$= 2J[\cos k_x + \cos k_y + \cos k_z] \qquad \text{(F-5)}$$

For the second neighbours let us first remark that we will have terms of the form, with a = 1:

$$\exp[i(k_\mu+k_\nu)]+\exp[i(k_\mu-k_\nu)]+\exp[i(-k_\mu+k_\nu)]+\exp[i(-k_\mu-k_\nu)] \tag{F-6}$$

where $\mu,\nu = x,y$ or z but $\mu \neq \nu$

$$= \exp(ik_\mu)\exp(ik_\nu)+\exp(ik_\mu)\exp(-ik_\nu)+\exp(-ik_\mu)\exp(ik_\nu) + \exp(-ik_\mu)\exp(-ik_\nu) \tag{F-7}$$

$$= 4\cos k_\mu \cos k_\nu . \tag{F-8}$$

The second neighbours contribution will consequently be:

$$4fJ\,[\cos k_x \cos k_y + \cos k_x \cos k_z + \cos k_y \cos k_z] . \tag{F-9}$$

With (F-9) and (F-5) in (13) (for a = 1),

$$J(k) = 2J\,[\cos k_x + \cos k_y + \cos k_z] + 4fJ\,[\cos k_x \cos k_y + \cos k_x \cos k_z + \cos k_y \cos k_z] \tag{F-10}$$

and (F-10) in (74) gives:

$$F_{sc} = (1/N)\sum_{\vec{k}}\left[1-(2[\cos k_x+\cos k_y+\cos k_z] +4f\,[\cos k_x\cos k_y+\cos k_x\cos k_z+\cos k_y\cos k_z])/(6+12f)\right]^{-1} \tag{F-11}$$

which is the Green's function for the simple cubic lattice including first and second neighbours values of F_{sc} as functions of f are given in the following Table F-1.

Table F-1

Green's function as a function of f. The numerical evaluation was made with the method described in Chapter 4. (extrapolating orders 3,4,5,6)

f	F_{sc}	f	F_{sc}
-.2	2.75145	.07	1.43292
-.15	2.04036	.08	1.42386
-.1	1.76064	.09	1.41533
-.09	1.72370	.1	1.40730
-.08	1.69071	.2	1.34706
-.07	1.66109	.3	1.30981
-.06	1.63434	.4	1.28511
-.05	1.61008	.5	1.26793
-.04	1.58798	.6	1.25557
-.03	1.56777	.7	1.24647
-.02	1.54923	.8	1.23964
-.01	1.53215	.9	1.23445
-1.E-9	1.516385445619	1.	1.23049
1.E-9	1.516385445619	2.	1.21910
.01	1.50178	3.	1.22213
.02	1.48822	4.	1.22721
.03	1.47561	5.	1.23231
.04	1.46385	6.	1.23700
.05	1.45286	7.	1.24123
.06	1.44257	8.	1.24503

Table F-1 cont'd.

f	F_{sc}	f	F_{sc}
9.	1.24843	3000.	1.33757
10.	1.25150	10000.	1.34186
15.	1.26332	30000.	1.34364
20.	1.27142	100000.	1.34434
30.	1.28210	300000.	1.34455
100.	1.30730	1000000.	1.34462
300.	1.32178	3000000.	1.34465
400.	1.32448	10000000.	1.34465
1000.	1.33132	100000000.	1.34466

The exact value (Watson 1939) is, for f = 0, 1.5163860 --- .

F-2: Body Centered Cubic Lattice

The first neighbours of site i in a BCC lattice are given by:

$$(\vec{R}_j - \vec{R}_i) = (\pm a/2, \pm a/2, \pm a/2) \qquad \text{(F-12)}$$

There are $z_1 = 8$ of them.

The second neighbours are given by:

$$(\vec{R}_k - \vec{R}_i) = \begin{matrix} (\pm a, 0, 0) \\ (0, \pm a, 0) \\ (0, 0, \pm a) \end{matrix}$$

There are $z_2 = 6$ of them.

One can remark, here, that the second neighbour structure of the BCC lattice is exactly the same as the SC first neighbour structure (see, e.g., equation (F-2)); the contribution of the second neighbours to $J(\vec{k})$ can be written directly from (F-5) with the proper coupling constant, and with a = 1:

$$2fJ\,(\cos k_n + \cos k_y + \cos k_z) \qquad \text{(F-13)}$$

The first neighbour contribution to the $J(\vec{k})$ is:

$$J \sum_{j=1^{st}\text{ neighbour}} \exp\left[i\vec{k}.(\vec{R}_j - \vec{R}_i)\right]$$

$$= J \quad \exp[\, i(k_x + k_y + k_z)/2] + \exp\,[\, i(k_x + k_y - k_z)/2]$$

$$+ \exp\,[\, i\,(k_x - k_y + k_z)/2 + \exp\,[\, i\,(k_x - k_y - k_z)/2]$$

$$+ \exp\,[\, i(-k_x + k_y + K_z)/2 + \exp\,[\, i\,(-k_x + k_y - K_z)/2]$$

$$+ \exp\,[\, i(-k_x - k_y + k_z)/2 + \exp\,[\, i\,(-k_x - k_y - k_z)/2] \qquad \text{(F-14)}$$

$$= J \quad [\, yz]\exp\,(ik_x/2) + [yx]\exp\,(-ik_x/2) \qquad \text{(F-15)}$$

where the symbol [yz) represents

$$\exp\,[\, i\,(k_y + k_z)/2] + \exp\,[\, i\,(k_y - k_z/2]$$

$$+ \exp\,[\, i\,(-k_y + k_z)/2] + \exp\,[\, i\,(-k_y - k_z)/2].$$

By factorization of [yz], (F-15) is:

$$J = \{[yz]\ 2\cos\,(k_x/2)\} \qquad \text{(F-16)}$$

By a similar process:

$[yz] = 2\cos\,(k_y/2)\ 2\cos\,(k_z/2)$; (F-17) and the contribution of the first neighbours to $J(\vec{k})$ is with (F-17) in (F-16):

$$8\,J\cos\,(k_x/2)\cos\,(k_y/2)\cos\,(k_z/2). \qquad \text{(F-18)}$$

Collecting (F-18), (F-13) in (74) one has,

$$F_{BCC} = (1/N) \sum_{\vec{k}} \Big[1-[\, 4 \cos (k_x/2) \cos (k_y/2)/ \cos (k_z/2) + f\, (\cos k_x + \cos k_y + \cos k_z)]/(4 + 3f) \Big]^{-1} \qquad \text{(F-19)}$$

The values of that function are given in Table F-2 as a function of f.

Table F-2

Green's function as a function of f for BCC lattice.

(orders 3,4,4,6 extrapolated)

f	F_{BCC}	f	F_{BCC}
-.6	1.86442	.05	1.38296
-.4	1.56395	.06	1.38106
-.3	1.49742	.07	1.37921
-.2	1.45152	.08	1.37741
-.15	1.43362	.09	1.37564
-.1	1.41821	.1	1.37392
-.09	1.41539	.2	1.35878
-.08	1.41265	.3	1.34670
-.07	1.40998	.4	1.33695
-.06	1.40738	.5	1.32901
-.05	1.40486	.6	1.32249
-.04	1.40240	.7	1.31711
-.03	1.40001	.8	1.31266
-.02	1.39768	.9	1.30896
-.01	1.39541	1.	1.30589
-.1.E-9	1.39320403023	2.	1.29390
1.E-9	1.39320402979	3.	1.29534
.01	1.39105	4.	1.30033
.02	1.38895	5.	1.30623
.03	1.38690	6.	1.31218
.04	1.38491	7.	1.31789

Table F-2 cont'd.

f	F_{BCC}	f	F_{BCC}
8.	1.32326	3000.	1.49927
9.	1.32827	10000.	1.50926
10.	1.33293	30000.	1.51370
15.	1.35190	100000.	1.51554
20.	1.36580	300000.	1.51610
30.	1.38512	1000000.	1.51630
100.	1.43463	3000000	1.51635
300.	1.46558	10000000.	1.51637
400.	1.47149	100000000.	1.51638
1000.	1.48609		

The exact value (Watson 1939) is, for f = 0, 1.3932039297 ---.

F - 3: Face Centered Cubic Lattice

The structure of the first neighbours of site i is given by:

$$\vec{R}_j - \vec{R}_i = \begin{matrix} (\pm a/2, \pm a/2, 0) \\ (\pm a/2, 0, \pm a/2) \\ (0 , \pm a/2, \pm a/2) \end{matrix} \qquad \text{(F-20)}$$

there are $z_1 = 12$ of them. The second neighbours of site i are given by:

$$\vec{R}_j - \vec{R}_i = \begin{matrix} (\pm a, 0, 0) \\ (0 , \pm a, 0) \\ (0 , 0, \pm a) \end{matrix} \qquad \text{(F-21)}$$

There are $z_2 = 6$ of them. One can readily see, comparing (F-21) with (F-2), that the structure of the second neighbour in the FCC lattice is identical with the SC lattice's first neighbour structure; their contribution to $J(\vec{k})$ is then, with a = 1, directly from (F-5):

$$2fJ (\cos k_x + \cos k_y + \cos k_z) . \qquad \text{(F-22)}$$

For the first neighbour contribution:

$$J \sum_{j=1}^{z_1} \exp\left[i\vec{k}.(\vec{R}_j - \vec{R}_i)\right]$$

$$= J \quad \exp\left[ia\,(k_x + k_y)/2\right] + \exp\left[ia\,(k_x - k_y)/2\right]$$

$$+ \exp\left[ia\,(-k_x + k_y)/2\right] + \exp\left[ia\,(-k_x - k_y)/2\right]$$

$$+ \exp\left[ia\,(-k_x + k_z)/2\right] + \exp\left[ia\,(-k_x - k_z)/2\right]$$

$$+ \exp\left[ia\,(-k_x + k_z)/2\right] + \exp\left[ia\,(-k_x - k_z)/2\right]$$

$$+ \exp\left[ia\,(\,k_y + k_z)/2\right] + \exp\left[ia\,(\,k_y - k_z)/2\right]$$

$$+ \exp\left[ia\,(-k_y + k_z)/2\right] + \exp\left[ia\,(-k_y - k_z)/2\right] \quad . \quad \text{(F-23)}$$

Collecting (F-22) and (F-24) in (74):

$$F_{FCC} = (1/N) \sum_{\vec{k}} \Big[1-[2(\cos k_x/2)\cos(k_y/2) + \cos(k_x/2)\cos(k_z/2)$$

$$+ \cos(k_y/2\cos(k_z/2)) + f(\cos k_x + \cos k_y + \cos k_z)]$$

$$/\,(6 + 3f) \Big]^{-1} \qquad \text{(F-25)}$$

The values of F_{FCC} are given in Table F-3.

Table F-3

Green's function as a function of f for FCC lattice.

(orders 3,4,5,6 exprapolated)

f	F_{FCC}	f	F_{FCC}
-.06	1.36096	.5	1.26365
-.05	1.35809	.6	1.25446
-.04	1.35528	.7	1.24665
-.03	1.35254	.8	1.24000
-.02	1.34985	.9	1.23430
-.01	1.34723	1.	1.22942
-1.E-9	1.344661145044	2.	1.20655
1.E-9	1.344661144536	3.	1.20414
.01	1.34214	4.	1.20819
.02	1.33968	5.	1.21449
.03	1.33727	6.	1.22149
.04	1.33490	7.	1.22855
.05	1.33259	8.	1.23540
.06	1.33033	9.	1.24194
.07	1.32811	10.	1.24812
.08	1.32593	15.	1.27409
.09	1.32380	20.	1.29367
.1	1.32172	30.	1.32140
.2	1.30296	100.	1.39414
.3	1.28745	300.	1.44026
.4	1.27452	400.	1.44909

Table F-3 cont'd

f	F_{FCC}	f	F_{FCC}
1000.	1.47095	300000.	1.51595
3000.	1.49072	1000000.	1.51625
10000.	1.50570	3000000.	1.51634
30000.	1.51236	10000000.	1.51637
100000.	1.51512	100000000.	1.51638
		1000000000.	1.51638

The exact value given by Watson (1939) is, for the case f = 0,

1.3446611832 ---.

Appendix G: Symmetrized Plane Waves for Cubic Lattices, First Few Functions

Symmetrized plane waves are difined by (102):

$$A_m(\vec{k}) = \sum_{|\vec{R}|=C_m} \exp[i\vec{k}.\vec{R}] \quad m = 1,2,... \quad (102)$$

To evaluate these summations we will need to know all the vectors, in a given lattice, having a given magnitude. We first describe the algorithm we need for that purpose and then give the results.

Then we derived the first few functions for the three cubic lattices. The lattice constant "a" is equal to 1 in every case. We treat the simple cubic case in some detail; for the other lattices, the calculation being very similar, we give only the results.

G - 2: Symmetrized Plane Waves

The vectors in the first shell, in a single cubic lattice, are, in units of a (see Table K-1):

$$\vec{R} = \begin{matrix} (\pm 1, 0, 0) \\ (0, \pm 1, 0) \\ (0, 0, \pm 1) \end{matrix} \quad (G\text{-}1)$$

and we have, with (G-1) in (102):

$$A_1(\vec{k}) = \exp(ik_x) + \exp(-ik_x) + \exp(ik_y) + \exp(-ik_y) + \exp(ik_z) + \exp(-ik_z)$$

or, using: $\cos x = [\exp(x) + \exp(-x)]/2$, (G-2)

$$A_1(\vec{k}) = 2(\cos k_x + \cos k_y + \cos k_z) \quad . \tag{G-3}$$

For m = 2 the vectors in the shell are; from Table K-1:

$$\vec{R} = \begin{matrix} (\pm 1, \pm 1, 0) \\ (\pm 1, 0, \pm 1) \\ (0, \pm 1, \pm 1) \end{matrix} \tag{G-4}$$

$$\begin{aligned} A_2(\vec{k}) = {} & \exp(ik_x)\exp(ik_y) + \exp(-ik_x)\exp(ik_y) \\ & + \exp(ik_x)\exp(-ik_y) + \exp(-ik_x)\exp(-ik_y) \\ & + \exp(ik_x)\exp(ik_z) + \exp(-ik_x)\exp(ik_z) \\ & + \exp(ik_x)\exp(-ik_z) + \exp(-ik_x)\exp(-ik_z) \\ & + \exp(ik_y)\exp(ik_z) + \exp(-ik_y)\exp(ik_z) \\ & + \exp(ik_y)\exp(-ik_z) + \exp(-ik_y)\exp(-ik_z) \end{aligned}$$

After factorization and using (G-2) it is:

$$A_2(\vec{k}) = 4(\cos k_x \cos k_y + \cos k_x \cos k_z + \cos k_y \cos k_z). \tag{G-5}$$

For m = 3, the vectors in the shell are, from Table K-1:

$$\vec{R} = (\pm 1, \pm 1, \pm 1) \tag{G-6}$$

(G-6) in (102) gives:

$$A_3(\vec{k}) = \exp[\, i(k_x + k_y + k_z)] + \exp\,[i(k_x + k_y - k_z)]$$
$$+ \exp[\, i(k_x - K_y + k_z)] + \exp\,[i(\, k_x - k_y - k_z)]$$
$$+ \exp[\, i(k_x - k_y + k_z)] + \exp\,[i(-k_x + k_y - K_z)]$$
$$+ \exp[i(-k_x - k_y + k_z)] + \exp[i(-k_x - k_y - k_z)] \qquad \text{(G-7)}$$

which is, after factorization and using (G-2),

$$A_3(\vec{k}) = 8 \cos k_x \cos k_y \cos k_z \qquad \text{(G-9)}$$

For m = 4 the vectors are

$$\vec{R} = \begin{matrix} (\pm 2, 0, 0) \\ (0, \pm 2, 0) \\ (0, 0, \pm 2) \end{matrix} \qquad \text{(G-10)}$$

The structure is the same as for m = 1 except for the ± 1;

consequently $A_4(\vec{k}) = 2\,(\cos 2k_x + \cos 2k_y + \cos 2k_z)$ (G-11)

For m = 5 the vectors are of a new symmetry type; for Table K-1:

$$\vec{R} = \begin{matrix} (\pm 1, \pm 2, 0) & \text{"xy pair"} \\ (\pm 2, \pm 1, 0) & \\ (\pm 1, 0, \pm 2) & \text{"xz pair"} \\ (\pm 2, 0, \pm 1) & \\ (0, \pm 1, \pm 2) & \text{"yz pair"} \\ (0, \pm 2, \pm 1) & \end{matrix} \qquad \text{(G-12)}$$

For the xy pair we have terms of the form

$$\exp [i(k_x + 2k_y)] + \exp [i(k_x - 2k_y)] + \exp [i(-k_x + 2k_y)]$$

$$+ \exp [i(-k_x - 2k_y)] + \exp [i(2k_x + k_y)] + \exp [i(2k_x - k_y)]$$

$$+ \exp [i(-2k_x + k_y)] + \exp [i(-2k_x - k_y)]$$

$$= 4 \ (\cos k_x \cos 2k_y + \cos 2k_x \cos k_y)$$

Consequently, with xz and yz pairs:

$$A_5(\vec{k}) = 4[\cos k_x \cos k_y + \cos 2k_x \cos k_y$$

$$+ \cos k_x \cos 2k_z + \cos 2k_x \cos k_z$$

$$+ \cos k_y \cos 2k_z + \cos 2k_y \cos k_z] \qquad \text{(G-13)}$$

For m = 6,

$$\vec{R} = \begin{matrix} (\pm 1, \pm 1, \pm 2) \\ (\pm 1, \pm 2, \pm 1) \\ (\pm 2, \pm 1, \pm 1) \end{matrix} \qquad \text{(G-14)}$$

and $A_6(\vec{k}) = 8 (\cos k_x \cos k_y \cos 2k_z + \cos k_x \cos 2k_y \cos k_z$

$$+ \cos 2k_x \cos k_y \cos k_z) + \qquad \text{(G-15)}$$

For m = 7,

$$\vec{R} = \begin{matrix} (\pm 2, \pm 2, 0) \\ (\pm 2, 0, \pm 2) \\ (0, \pm 2, \pm 2) \end{matrix} \qquad \text{(G-16)}$$

and $A_7(\vec{k}) = 4\,[\cos 2k_x \cos 2k_y + \cos 2k_x \cos 2k_z + \cos 2k_y \cos 2k_z]$. (G-17)

For m = 8

$$\vec{R} = \begin{matrix} (\pm 2, \pm 2, \pm 1) \\ (\pm 2, \pm 1, \pm 2) \\ (\pm 1, \pm 2, \pm 2) \\ (\pm 3, 0, 0) \\ (0, 0, \pm 3) \end{matrix} \qquad \text{(G-16)}$$

and $A_8(\vec{k}) = 8\,[\cos 2k_x \cos 2k_y \cos k_z + \cos 2k_x \cos k_y \cos 2k_z + \cos k_x \cos 2k_y \cos k_z]$

$$+ 2\,(\cos 3k_x + \cos 3k_y + \cos 3k_z)\,. \qquad \text{(G-19)}$$

and so on.

FCC Symmetrized plane waves

For m = 1, from Table (K-2), in units of a:

$$\vec{R} = \begin{matrix} (\pm 1/2, \pm 1/2, 0) \\ (\pm 1/2, 0, \pm 1/2) \\ (0, \pm 1/2, \pm 1/2) \end{matrix} \qquad \text{(G-20)}$$

and $A_1(\vec{k}) = \exp [i (k_x + k_y)/z] + \exp [i (k_x - k_y)/2]$

$+ \exp[i (-k_x + k_y)/2] + \exp [i (-k_x - k_y)/2] + \exp [i (k_x + k_y)/2]$

$+ \exp[i (k_x - k_z)/2] + \exp [i (-k_x - k_z)/2] + \exp [i (-k_x - k_z)/2]$

$+ \exp[i (k_y + k_z)/2] + \exp [i (k_y - k_z)/2] + \exp [i (-k_y + k_z)/2]$

$+ \exp [i (-k_y - k_z)/2]$

or,

$$A_1(\vec{k}) = 2[\cos(k_x/2) \cos(k_y/2) + \cos(k_z/2) + \cos(k_y/2) \cos(k_z/2)] \qquad \text{(G-21)}$$

For m = 2

$$\vec{R} = \begin{matrix} (\pm, 0, 0) \\ (0, \pm 1, 0) \\ (0, 0, \pm 1) \end{matrix} \qquad \text{(G-22)}$$

which is the same situation as m = 1 in SC, therefore,

$$A_2(\vec{k}) = 2(\cos k_x + \cos k_y + \cos k_z) . \qquad \text{(G-23)}$$

For m = 3

$$\vec{R} = \begin{matrix} (\pm 1, \pm 1/2, \pm 1/2) \\ (\pm 1/2, \pm 1, \pm 1/2) \\ (\pm 1/2, \pm 1/2, \pm 1) \end{matrix} \qquad \text{(G-24)}$$

which gives, in a similar fashion as for m = 6 in SC,

$$A_3(\vec{k}) = 8\,[\cos k_x \cos(k_y/2) \cos(k_z/2) + \cos(k_x/2) \cos k_y \cos(k_z/2) + \cos(k_x/2) \cos(k_y/2) \cos k_z) \quad \text{(G-25)}$$

For m = 4 (in units of a)

$$\vec{R} = \begin{matrix} (\pm 1, \pm 1, 0) \\ (\pm 1, 0, \pm 1) \\ (0, \pm 1, \pm 1) \end{matrix} \quad \text{(G-26)}$$

The situation is identical with m = 2 in SC.

Therefore,

$$A_4(\vec{k}) = 4\,(\cos k_x \cos k_y + \cos k_x \cos k_z + \cos k_y \cos k_z) \quad \text{(G-27)}$$

For m = 5

$$\vec{R} = \begin{matrix} (\pm 3/2, \pm 1/2, 0) \\ (\pm 1/2, \pm 3/2, 0) \\ (\pm 3/2, 0, \pm 1/2) \\ (\pm 1/2, 0, \pm 3/2) \\ (0, \pm 3/2, \pm 1/2) \\ (0, \pm 1/2, \pm 3/2) \end{matrix} \quad \text{(G-28)}$$

The situation is similar to m = 5 in SC and, by analogy with (G-13),

$$A_5(\vec{k}) = 4\,[\cos(3k_x/2)\cos(k_y/2) + \cos(k_x/2)\cos(3k_y/2) + \cos(3k_x/2)\cos(k_z/2) + \cos(k_x/2)\cos(3k_z/2) + \cos(3k_y/2)\cos(k_z/2) + \cos(k_y/2)\cos(3k_z/2)] \quad \text{(G-29)}$$

For m = 6

$$\vec{R} = (\pm 1, \pm 1, \pm 1) \quad \text{(G-30)}$$

As for m = 3 in SC,

$$A_6(\vec{k}) = 8 \cos k_x \cos k_y \cos k_z \quad \text{(G-31)}$$

For m = 7

$$\vec{R} = \begin{matrix} (\pm 3/2, \pm 1, \pm 1/2) \\ (\pm 1, \pm 3/2, \pm 1/2) \\ (\pm 1, \pm 1/2, \pm 3/2) \\ (\pm 1/2, \pm 1, \pm 3/2) \\ (\pm 1/2, \pm 3/2, \pm 1) \\ (\pm 3/2, \pm 1/2, \pm 1) \end{matrix} \quad \text{(G-32)}$$

and, after substitution into (102)

$$A_7(\vec{k}) = 8\,[\cos(3k_x/2)\cos k_y \cos(k_z/2) + \cos(k_x/2)\cos(3k_y/2)\cos k_z + \cos k_x \cos(k_y/2)\cos(3k_z/2) + \cos(k_x/2)\cos k_y \cos(3k_z/2) + \cos(3k_x/2)\cos(k_y/2)\cos(k_z) + \cos k_x \cos(3k_y/2)\cos(k_z\ 2)] \qquad \text{(G-33)}$$

For m = 8, in units of a:

$$\vec{R} = \begin{matrix} (\pm, 0, 0) \\ (0, \pm 2, 0) \\ (0, 0, \pm 2) \end{matrix} \qquad \text{(G-34)}$$

which has the same symmetry as m = 1 in SC, consequently, replacing $\vec{k}$ by $2\vec{k}$ in (G-3):

$$A_8(\vec{k}) = 2(\cos 2k_x + \cos 2k_y + \cos 2k_z). \qquad \text{(G-35)}$$

For m = 9

$$\vec{R} = \begin{matrix} (\pm 3, \pm 3, 0) \\ (\pm 3, 0, \pm 3) \\ (0, \pm 3, \pm 3) \\ (\pm 4, \pm 1, \pm 1) \\ (\pm 1, \pm 4, \pm 1) \\ (\pm 1\ \pm 1\ \pm 4) \end{matrix} \qquad \text{(G-36)}$$

The first three points have the m = 4 (FCC) symmetry and the last three points have the m = 3 (FCC) symmetry; therefore, using (G-27) and (G-25):

$$A_9(\vec{k}) = 4\,[\cos(3k_x/2)\cos(3k_y/2) + \cos(3k_x/2)\cos(3k_z/2) + \cos(3k_y/2)\cos(3k_z/2)] + 8[\cos(2k_x)\cos(k_y/2)\cos(k_z/2) + \cos(k_x/2)\cos(2k_y)\cos(k_z/2) + \cos(k_x/2)\cos(k_y/2)\cos(2k_z)] \quad \text{(G-37)}$$

BCC Symmetrized Plane Waves.

Following the same procedures as for SC and FCC lattices one has:

$$A_1(\vec{k}) = 4\,[\cos(k_x/2)\cos(k_y/2) + \cos(k_x/2)\cos(k_z/2) + \cos(k_y/2)\cos(k_z/2)] \quad \text{(G-38)}$$

$$A_2(\vec{k}) = 2[\cos k_x + \cos k_y + \cos k_z] \quad \text{(G-39)}$$

$$A_3(\vec{k}) = 8[\cos k_x \cos(k_y/2)\cos(k_z/2) + \cos(k_x/2)\cos k_y \cos(k_z/2) + \cos(k_x/2)\cos(k_y/2)\cos k_z] \quad \text{(G-40)}$$

$$A_4(\vec{k}) = 4[\cos k_x \cos k_y + \cos k_x \cos k_z + \cos k_y \cos k_z] \quad \text{(G-41)}$$

$$A_5(\vec{k}) = 4[\cos(3k_x/2)\cos(k_y/2) + \cos(k_x/2)\cos(3k_y/2)$$

$$+ \cos(3k_x/2)\cos(k_y/2) + \cos(k_x/2)\cos(3k_z/2)$$

$$+ \cos(3k_y/2)\cos(k_z/2) + \cos(k_y/2)\cos(3k_z/2)] \qquad \text{(G-42)}$$

$$A_6(\vec{k}) = 8\cos k_x \cos k_y \cos k_z \qquad \text{(G-43)}$$

$$A_7(\vec{k}) = 8\cos(3k_x/2)\cos k_y \cos(k_z/2) + \cos(k_x/2)\cos(3k_y/2)\cos k_z$$

$$+ \cos k_x \cos(k_y/2)\cos(3k_z/2) + \cos(k_x/2)\cos k_y \cos(3k_z/2)$$

$$+ \cos(3k_x/2)\cos(k_y/2)\cos k_z + \cos k_x \cos(3k_y/2)\cos(k_z/2)]$$

$$\text{(G-44)}$$

$$A_8(\vec{k}) = 2[\cos(2k_x) + \cos(2k_y) + \cos(2k_z)] \qquad \text{(G-45)}$$

Appendix H: Cubic Point Group Operations

We give here a quick way to get the cubic point group representations in 3 x 3 matrices as needed in the Chadi and Cohen method.

Starting with the point (a,b,c) (see Figure H-1) and considering the plane reflections through plans xy and nz one gets the points (a,b,-c) and (a,-b,c); reflection of one of these points through the same plane leads to the point (a,-b,-c). The four points obtained belong to the symmetry sub-group of the point (a,b,c) as well as the points generated if we rotate that rectangle around the n ones by 90 degrees. We have, in fact, the eight symmetry points of (b,c) in the two dimension square lattice symmetry. The three dimensional cubic symmetry also involves rotations around y and z ones. Rotating the first 8 points around the y ones by 90, 180 and 270 degrees we get the subgroups SGI. SGII and SGIII successively. Rotations by the same angles around the z ones generate the sub-groups SGIV,SGII and SGV. Reflection through any plane (of the cubic symmetry) will generate no new point. We then have the whole set of symmetric points of (a,b,c) according to the cubic or octahedral symmetry. The operations of the cubic symmetry point group are then simply the operations relating any of the 48 points generated to the point (a,b,c). They are easily written directly from Figure G-1; for example the matrix transforming

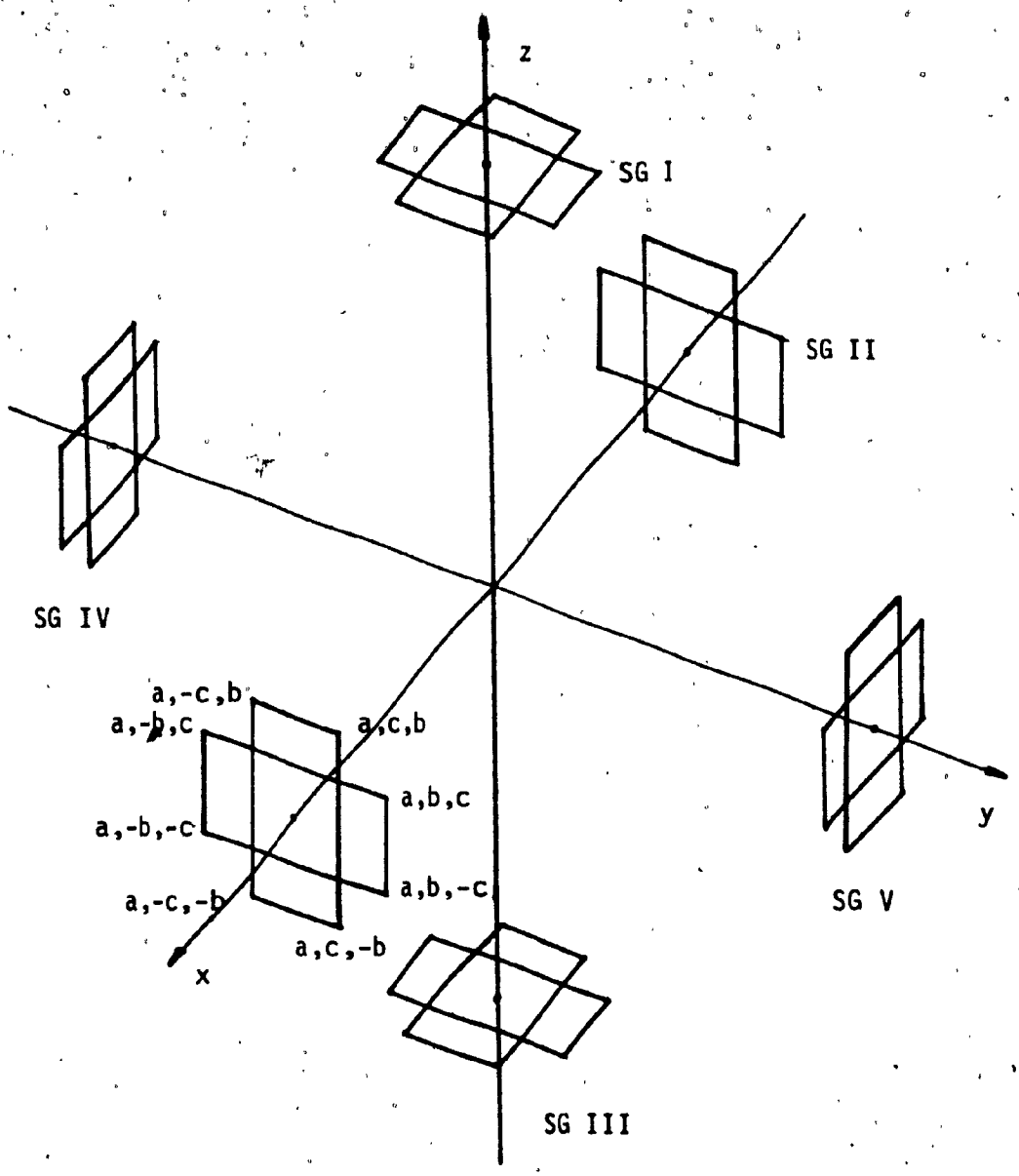

Fig H-1

(a,b,c) to (c,-b,a) is

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} c \\ -b \\ a \end{pmatrix}.$$

the whole set of matrices T_i is:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

the whole set of matrices T_i cont'd.

$$\begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & -0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Appendix I: First Brillouin Zone of Body Centered Cubic Lattice.

The BCC first Brillouin zone has the shape, see Aschroft & Mermin (1979); in units of $\frac{2\pi}{a}$.

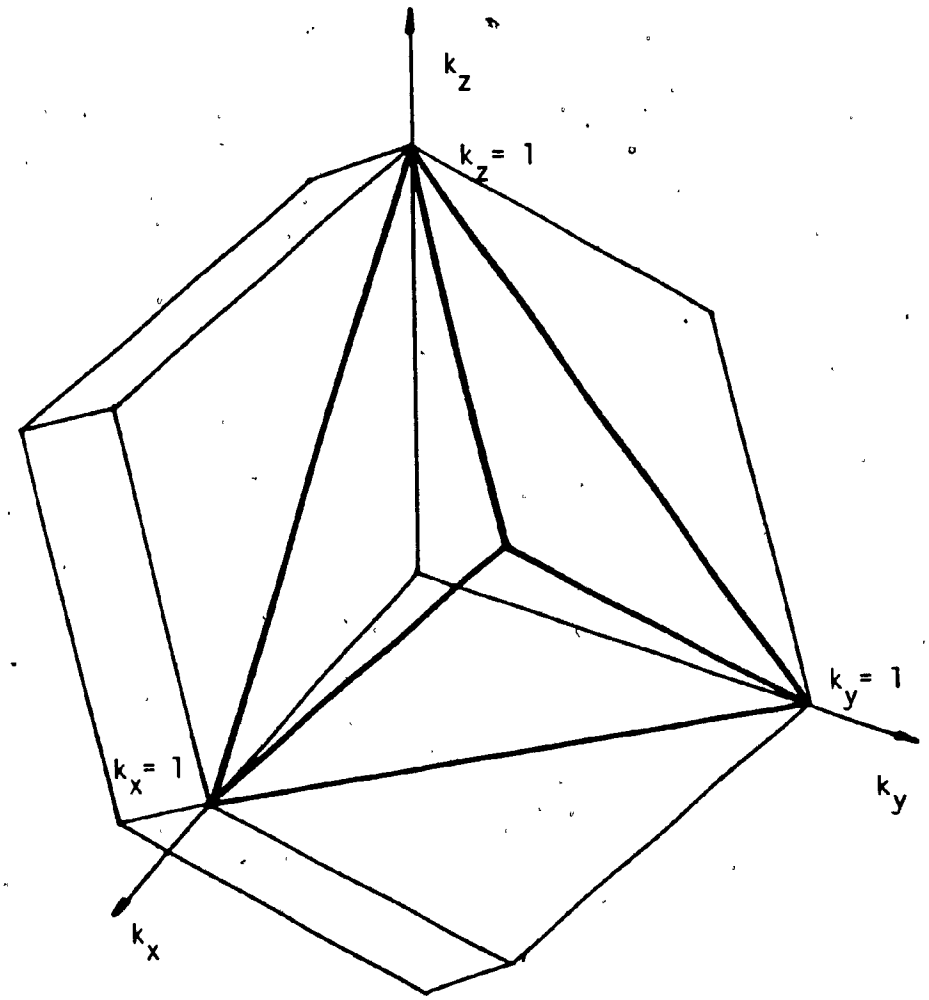

Fig I-1

Considering only the so called irreducible Brillouin zone, the part of the zone with all positive coordinates:

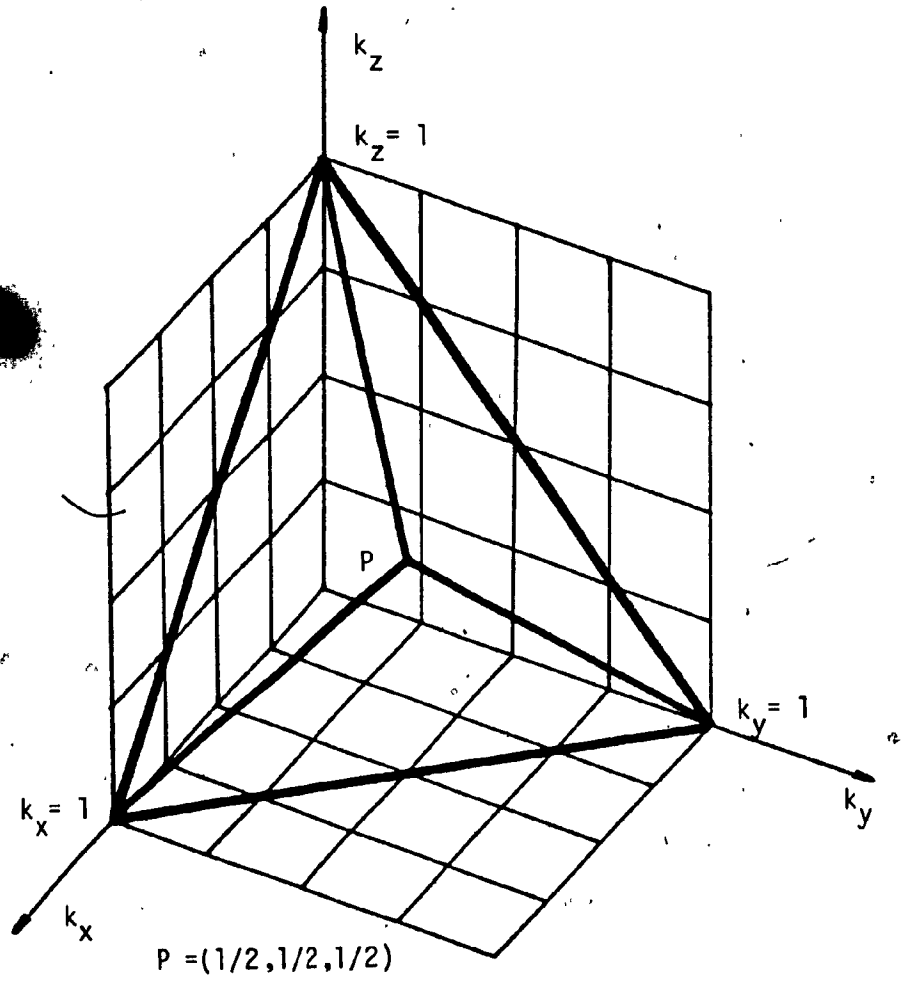

Fig I-2

the plane defined by the points (1,0,0), (0,1,0) and (1/2, 1/2, 1/2) is defined by equation $x + y = 1$. The region of space on the same side, of that plane, as the origin (and including that plane) is defined by the inequality

$$x + y \leq 1. \qquad \text{(I-1)}$$

Similarly one can write, for the points (1,0,0), (0,0,1) and (1/2, 1/2, 1/2):

$$x + z \leq 1 \qquad \text{(I-2)}$$

and for the points (0,1,0), (0,0,1), (1/2, 1/2, 1/2):

$$y + z \leq 1 \quad . \qquad \text{(I-3)}$$

The irreducible Brillouin zone is, therefore defined by the three simultaneous inequalities (I-1), (I-2) and (I-3). The complete Brillouin zone is defined by (x, y and z are in $2\pi/a$ units)

$$\begin{aligned} |x| + |y| &\leq 1 \\ |x| + |z| &\leq 1 \\ |y| + |z| &\leq 1 \end{aligned} \qquad \text{(I-4)}$$

Appendix J: Analytical Geometry Description of the First Brillouin Zone of the FCC lattice.

The irreducible (all coordinates positive) part of FCC Brillouin zone can be seen in Figures J-1 and J-2 since the FCC is the intersection of a cube, with faces parallel to the ones and of side 2 (in units of $2\pi/a$) and of an octahedron with vertices at $\pm \frac{3}{2}$ (in units of $2\pi/a$ on each axis).

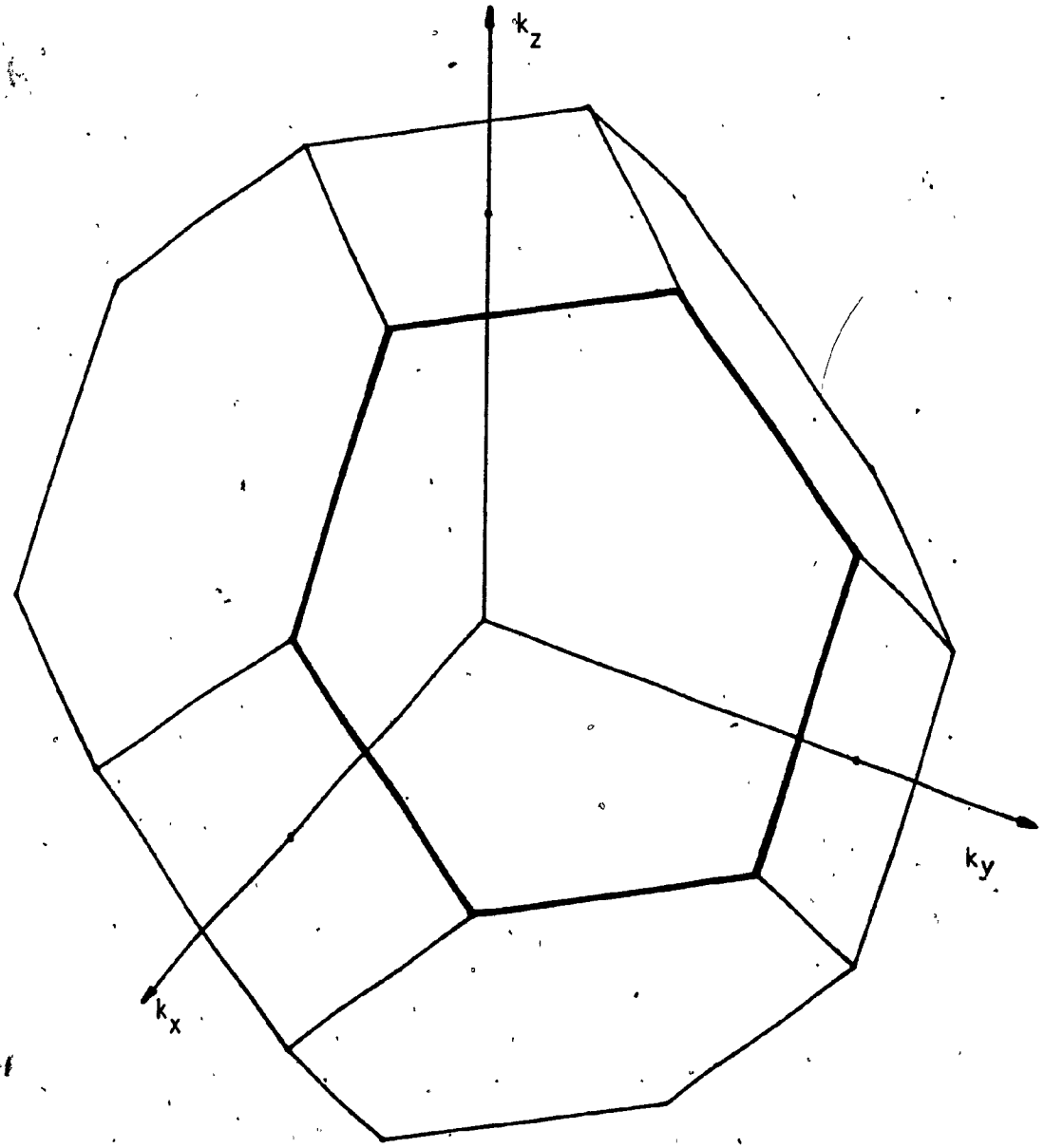

Fig J-1

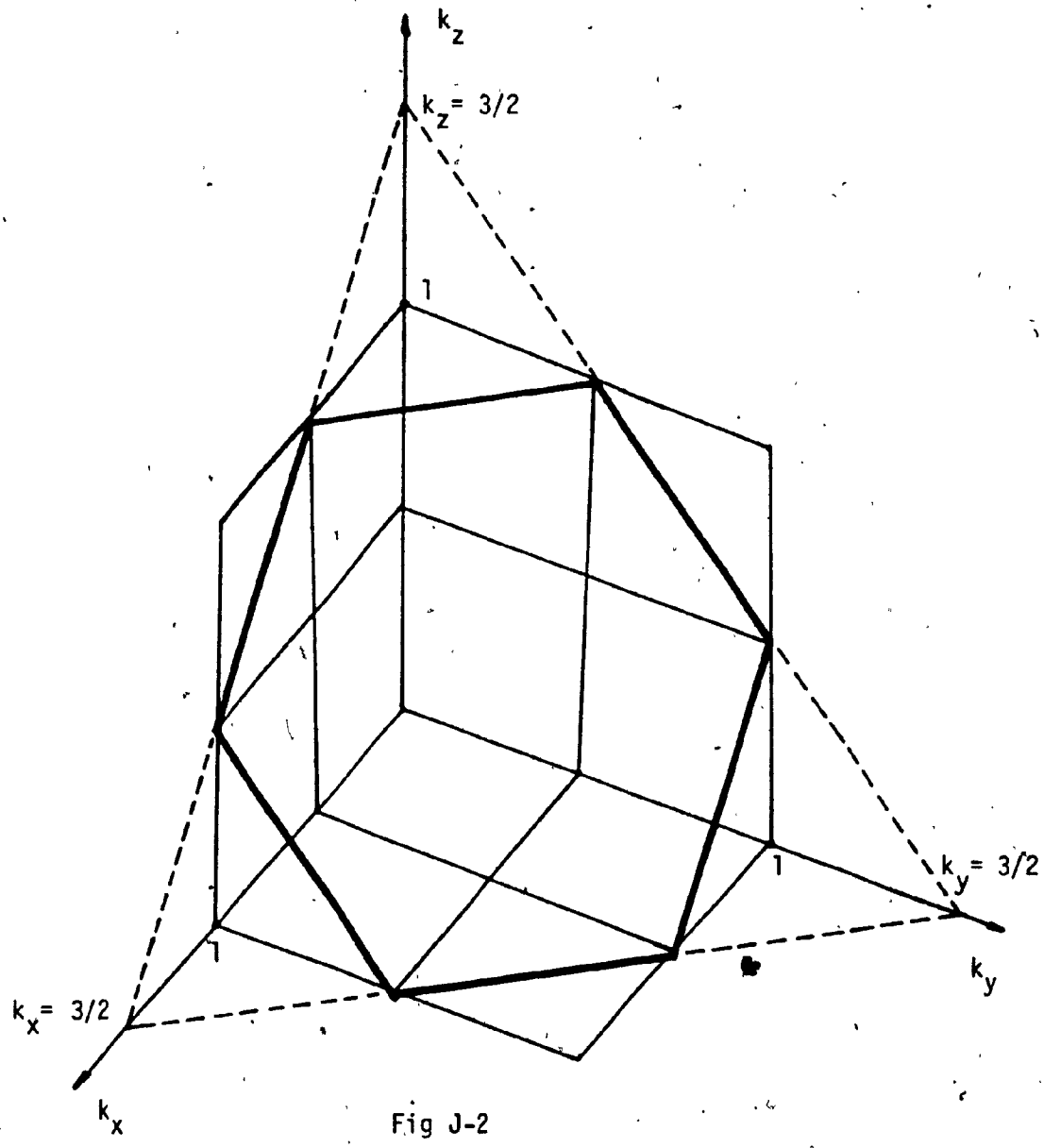

Fig J-2

to be inside the cube a point (x, y, z) must satisfy (in units of $2\pi/a$)

$$\begin{aligned} |x| &\leq 1 \\ |y| &\leq 1 \\ |z| &\leq 1 \end{aligned} \qquad \text{(J-1)}$$

and to be inside the octahedron and the condition is (in units of $2\pi/a$)

$$|x| + |y| + |z| \leq 3/2 \qquad \text{(J-2)}$$

since, for the irreducible BZ, the octahedron part is limited by the plane $x + y + z = 3/2$ or can be seen directly from Figure I-1. The condition that (x, y, z) must satisfy to belong to the FCC and BZ as (J-1) and (J-2) together.

Appendix K: Cubic Lattices

We collecthere some useful properties of the cubic lattices used throughout this thesis.

K-1: Number of Sites at a Given Distance from the Origin in Cubic Lattices.

A Bravais lattice is defined by (Ashcroft & Mermin Chapter 4):

$$\vec{R} = n_1 a_1 + n_2 + n_3 a_3 \qquad \text{(K-1)}$$

where n_1, n_2, n_3 are integers, a_i are basis vector of the lattice:

$$a_i = x_i \vec{i} + y_i \vec{j} + z_i \vec{k} \qquad \text{(K-2)}$$

x_i y_i z_i are real numbers and $\vec{i}$, $\vec{j}$, $\vec{k}$ are the usual Cartesian unit vectors.

The distance, in any Bravais lattice, between the origin and a given site characterized by $\vec{R}$ is given by:

$$|\vec{R}|^2 = (n_1 x_1 + n_2 x_2 + n_3 x_3)^2 + (n_1 y_1 + n_2 y_2 + n_3 y_3)^2$$

$$+ (n_1 z_1 + n_2 z_2 + n_3 z_3)^2 \qquad \text{(K-3)}.$$

In the simple cubic lattice, the basis vectors are usually taken to be:

$$(n_i\ y_i\ z_i) = \begin{matrix} (\ a,\ 0,\ 0\ ) \\ (\ 0,\ a,\ 0\ ) \\ (\ 0,\ 0,\ a\ ) \end{matrix} \qquad \text{(K-4)}$$

where a is the lattice constant.

which gives for the distance between the point $(n_1 a,\ n_2 a,\ n_3 a)$ and the origin:

$$|\vec{R}|^2 = a^2\ (n_1^2 + n_2^2 + n_3^2)\ . \qquad \text{(K-5)}$$

Since n_1, n_2, n_3 are integers $n_1^2 + n_2^2 + n_3^2$ will also be an integer. The number of points at a given distance in a simple cubic lattice is then equal to the number of ways to obtain a particular integer ($|\vec{R}|^2 / a^2$) as a sum of squares of other integers. For example if one wants to know the number of neighbours at a distance $\sqrt{3}$ a in a simple cubic lattice one simply has to find all the integer solutions of the Diophantine equation:

$$3 = n_1^2 + n_2^2 + n_3^2$$

the obvious result is $n_1 = n_2 = n_3 = \pm 1$

which gives 8 different solutions in all; and there are 8 sites at distance $\sqrt{3}$ a from origin in SC.

The computer algorithm we used is to search, in loops, all solutions of such equations and to count them.

The Diophantine's equations for the two other cubic lattices are, for BCC, taking

$$\vec{a}_1 = a\vec{i} \quad \vec{a}_2 = a\vec{j} \quad \vec{a}_3 = (a/2)(\vec{i} + \vec{j} + \vec{k})$$

$$\frac{4\,|\vec{R}|^2}{a^2} = 4n_1^2 + 4n_2^2 + 3n_3^2 + 4n_1 n_3 + 4n_2 n_3 \qquad \text{(K-6)}$$

and for FCC, taking

$$\vec{a}_1 = \frac{a}{2}(\vec{i} + \vec{j})$$

$$\vec{a}_2 = \frac{a}{2}(\vec{j} + \vec{k})$$

$$\vec{a}_3 = \frac{a}{2}(\vec{i} + \vec{k})$$

$$2\,|R^2| = n_1^2 + n_2^2 + n_3^2 + n_1 n_2 + n_1 n_3 + n_2 n_3 \,. \qquad \text{(K-7)}$$

Results are in the following three tables. Typical points are all positive number solutions encountered in the process; all solutions can be generated from these points by application of the cubic point groups symmetry operators given in Appendix H.

Table K-1

Simple Cubic Lattice

$\frac{\vec{R}^2}{a^2}$	Number of Sites	Typical Point (s) in Units of a
1	6	(1, 0, 0)
2	12	(1, 1, 0)
3	8	(1, 1, 1)
4	6	(2, 0, 0)
5	24	(2, 1, 0)
6	24	(2, 1, 1)
7	0	-
8	12	(2, 2, 0)
9	30	(2, 2, 1) (3, 0, 0)
10	24	(3, 1, 0)
11	24	(3, 1, 1)
12	8	(2, 2, 2)
13	24	(3, 2, 0)
14	48	(3, 2, 1)
15	0	-
16 14th shell	6	(4, 0, 0)
17	48	(4, 1, 0) (3, 2, 2)
18	36	(4, 1, 1) (3, 3, 0)
19	24	(3, 3, 1)
20 18th shell	24	(4, 2, 0)

Table K-1

Simple Cubic Lattice cont'd

$\frac{\lvert\vec{R}\rvert^2}{a^2}$	Number of Sites	Typical Point(s)
21	48	(4, 2, 1)
22	24	(3, 3, 2)
23	0	-
24	24	(4, 2, 2)
25	30 (22nd shell)	(4, 3, 0) (5, 0, 0)
26	72	(4, 3, 1) (5, 1, 0)
27	32	(3, 3, 3) (5, 1, 1)
28	0	-
29	72	(4, 3, 2) (5, 2, 0)
30	48 (26th shell)	(5, 2, 1)
31	0	-
32	12	(4, 4, 0)
33	48	(4, 4, 1) (5, 2, 2)
34	48	(4, 3, 3) (5, 3, 0)
35	48 (30th shell)	(5, 3, 1)
36	30	(4, 4, 2) (6, 0, 0)
37	24	(6, 1, 0) -
38	72	(5, 3, 2) (6, 1, 1)
39	0	-
40	24 (34th shell)	(6, 2, 0)
41	96	(6, 2, 1)(5,4,0)(4,4,3)
42	48	(5, 4, 1)
43	24	(5, 3, 3)
44	24	(6, 2, 2)
45	72 (39th shell)	(5, 4, 2) (6, 3, 0)

Table K-1

Simple Cubic Lattice cont'd

$\frac{\lvert R\rvert^2}{a^2}$	Number of Sites	Typical Points
46	48	(6,3,1)
47	0	-
48	8 (41st shell)	(4,4,4)
49	54	(6,3,2)(7,0,0)
50	84	(5,4,3)(5,5,0)(7,1,0)
51	48	(5,5,1)(7,1,1)
52	24	(6,4,0)
53	72	(7,2,0)(6,4,1)
54	96	(7,2,1)(5,5,2)(6,3,3)
55	0	-
56	48	(6,4,2)
57	48	(5,4,4)(7,2,2)
58	24	(7,3,0)
59	72	(7,3,1)(5,5,3)
60	0	-
61	72	(6,4,3)(6,5,0)
62	96	(7,3,2)(6,5,1)
63	0	-
64	6	(8,0,0)
65	96	(8,1,0)(7,4,0)(6,5,2)

Table K-1

Simple Cubic Lattice cont'd

$\frac{\lvert R\rvert^2}{a^2}$	Number of Sites	Typical Points
66	96	(8,1,1)(7,4,1)(5,5,4)
67	24	(7,3,3)
68	48	(6,4,4)(8,2,0)
69	96	(8,2,1)(7,4,2)
70	48	(6,5,3)
71	0	-
72	36	(6,6,0)(8,2,2)
73	48	(6,6,1)(8,3,0)
74	120	(7,4,3)(7,5,0)(8,3,1)
75	56	(5,5,5)(7,5,1)
76	24	(6,6,2)
77	96	(6,5,4)(8,3,2)
78	48	(7,5,2)
79	0	-
80	24	(8,4,0)

Table K-1

Simple Cubic Lattice cont'd

$\frac{\vec{R}_i^2}{a^2}$	Number of Sites	Typical Point(s)
81	102	(6,6,3)(7,4,4)(8,4,1)(9,0,0)
82	48	(8,3,3)(9,1,0)
83	72	(7,5,3)(9,1,1)
84	48	(8,4,2)
85	48	(7,6,0)(9,2,0)
86	120	(6,5,5)(7,6,1)(9,2,1)
87	0	-
88	24	(6,6,4)
89	144	(7,6,2)(8,4,3)(8,5,0)(9,2,2)
90	120	(7,5,4)(8,5,1)(9,3,0)
91	48	(9,3,1)
92	0	-
93	48	(8,5,2)
94	96	(7,6,3)(9,3,2)
95	0	-
96	24	(8,4,4)
97	48	(6,6,5)(9,4,0)
98	108	(7,7,0)(8,5,3)(9,4,1)
99	72	(7,5,5)(7,7,1)(9,3,3)
100	30	(8,6,0)(10,0,0)

Table K-2

Face Centered Cubic Lattice

$\frac{\lvert\vec{R}\rvert^2}{a^2}$	Number of Sites	Typical Point (s) in Unites of (a/2)
0.5	12	(1, 1, 0)
1	6	(2, 0, 0)
1.5	24	(2, 1, 1)
2	12	(2, 2, 0)
2.5	24	(3, 1, 0)
3	8	(2, 2, 2)
3.5	48	(3, 2, 1)
4	6	(4, 0, 0)
4.5	36	(3, 3, 0) (4, 1, 1)
5	24	(4, 2, 0)
5.5	24	(3, 3, 2)
6	24	(4, 2, 2)
6.5	72	(4, 3, 1) (5, 1, 0)
7	0	
7.5	48	(5, 2, 1)
8	12	(4, 4, 0)
8.5	48	(5, 3, 0) (4, 3. 3)
9	30	(4, 4, 2) (6, 0, 0)
9.5	72	(5, 3, 2) (6, 1, 1)
10	24	(6, 2, 0)

Table K-3

Body Centered Cubic Lattice

$\frac{\vec{R}^2}{a^2}$	Number of Sites	Typical Point(s) in Units of (a/2)
0.75	8	(1, 1, 1)
1	6	(2, 0, 0)
2	12	(2, 2, 0)
2.75	24	(3, 1, 1)
3	8	(2, 2, 2)
4	6	(4, 0, 0)
4.75	24	(3, 3, 1)
5	24	(4, 2, 0)
6	24	(4, 2, 2)
6.75	32	(3, 3, 3) (5, 1, 1)
8	12	(4, 4, 0)
8.25	48	(5, 3, 1)
9	30	(4, 4, 2) (6, 0, 0)
10	24	(6, 2, 0)
10.75	24	(5, 3, 3)
11	24	(6, 2, 2)
12	8	(4, 4, 4)
12.75	48	(7, 1, 1) (5, 5, 1)
13	24	(6, 4, 0)
14	48	(6, 4, 2)
14.75	72	(5, 5, 3) (7, 3, 1)

Number of Points in Cubic Subgroups

If the absolute values of the coordinates of a point are all equal, that point belongs to a subgroup of the cubic point group containing 8 points as can be seen directly in figure K-1.

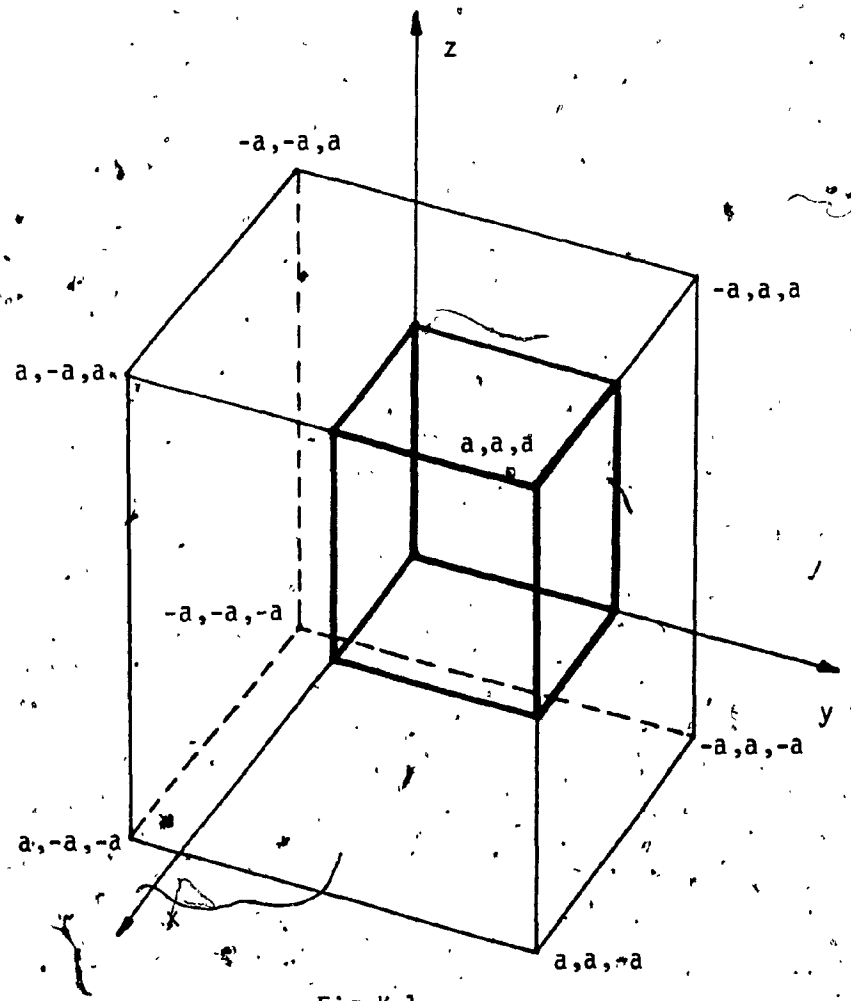

Fig K-1

If the absolute values of two coordinates of a point are equal (with the third being different) that point belongs to a cubic symmetry subgroup containing 24 points (see figure (K-2).

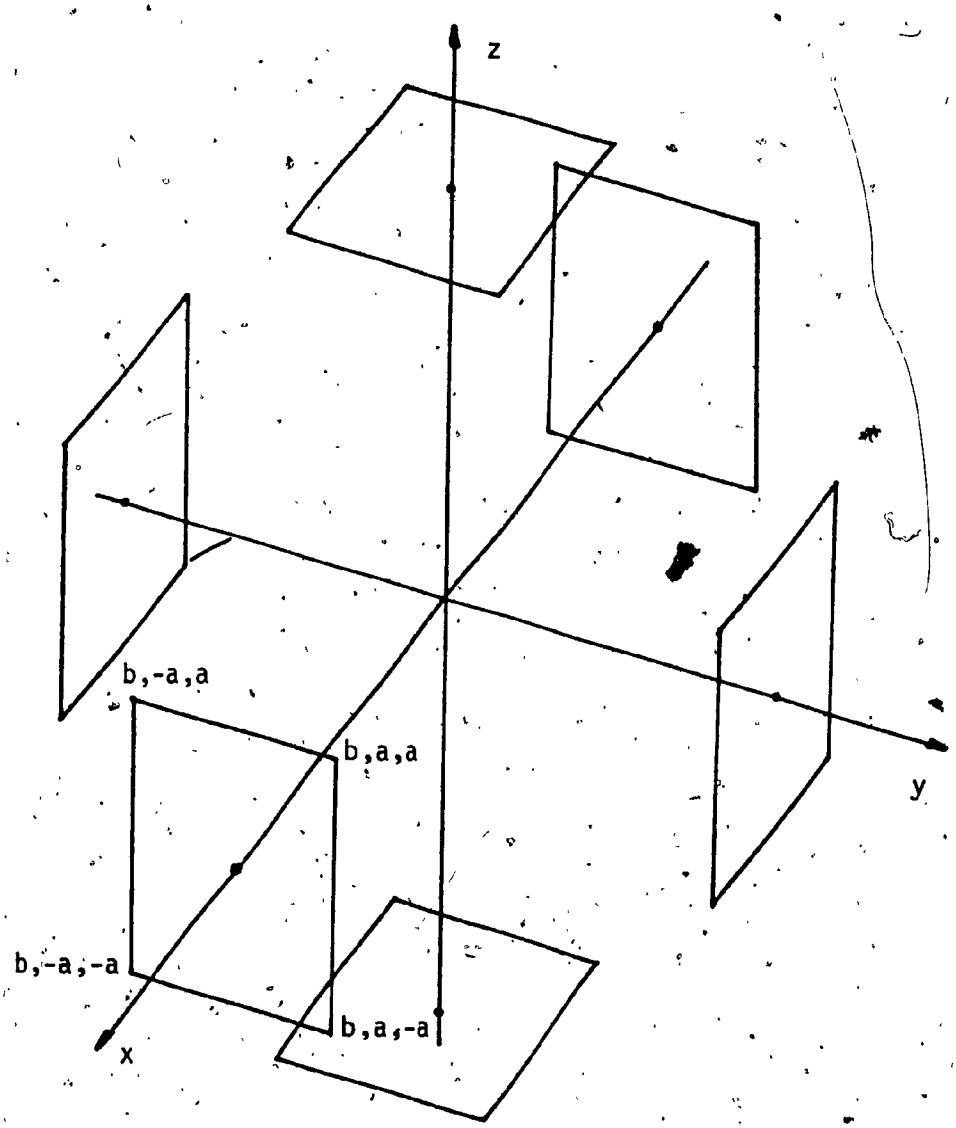

Fig K-2

If the absolute values of the 3 coordinates of a point are all different then that point belongs to the subgroup of the cubic point group which contain 48 elements i.e., which is the cubic point group itself.

```
      PROGRAM FSC (INPUT,OUTPUT)
C
C
C
      DIMENSION C(2000),G(4),X(4),DN(4,4),DD(4,4)
10    CONTINUE
      PI=3.141592654
      NN=3
C NN IS THE STARTING ORDER
      READ *,F
      IF (F-1.1E+9) 15,20,20
15    DO 102 III=1,4,1
      N=NN+III-1
      TH=PI/((2.0**N)*2.0)
      LI=(2*(2**N))-1
      DO 6 M=1,LI,2
      C(M)=COS(TH*M)
6     CONTINUE
      CALL CALC(LI,NU,C,F,GREEN)
      G(III)=GREEN
      X(III)=1.00/LI
102   CONTINUE
      DO 105 LL=1,4,1
      DN(LL,1)=X(LL)**3
      DD(LL,1)=DN(LL,1)
      DN(LL,2)=X(LL)*X(LL)
      DD(LL,2)=DN(LL,2)
      DN(LL,3)=X(LL)
      DD(LL,3)=X(LL)
      DN(LL,4)=G(LL)
      DD(LL,4)=1.0
105   CONTINUE
      CALL DET4(DN,RN)
      CALL DET4(DD,RD)
      FF1=RN/RD
      T2=0.25*(1.0-(1.0/FF1))
      PRINT *,F,FF1,T2
      GO TO 10
20    CONTINUE
      END
      SUBROUTINE CALC(LI,NU,C,F,FF)
      DIMENSION C(2000)
      SU=0.0
      NU=0
      DE=3.0+6.0*F
      DO 1 I=1,LI,2
      CI=C(I)
      DO 1 J=I,LI,2
      CJ=C(J)
      DO 1 K=J,LI,2
```

```
      CK=C(K)
      IF((I.EQ.J).AND.(I.EQ.K).AND.(J.EQ.K)) GO TO 2
      IF((I.EQ.J).OR.(I.EQ.K).OR.(J.EQ.K)) GO TO 3
      AL=6
      GO TO 4
2     AL=1
      GO TO 4
3     AL=3
4     CONTINUE
      AA=CI+CJ+CK
      BB=2.0*F*((CI*CJ)+(CI*CK)+(CJ*CK))
      RJJ=(AA+BB)/DE
      TE=AL/(1.0-RJJ)
      NU=NU+AL
      SU=SU+TE
1     CONTINUE
      FF=SU/(NU*1.0)
      RETURN
      END
      SUBROUTINE DET4(DD,R)
      REAL J,I,K,L,M,N
      DIMENSION DD(4,4)
C
      A=DD(1,1)
      B=DD(1,2)
      C=DD(1,3)
      D=DD(1,4)
C
      E=DD(2,1)
      F=DD(2,2)
      G=DD(2,3)
      H=DD(2,4)
C
      I=DD(3,1)
      J=DD(3,2)
      K=DD(3,3)
      L=DD(3,4)
C
      M=DD(4,1)
      N=DD(4,2)
      O=DD(4,3)
      P=DD(4,4)
C
      P1=(A*F-B*E)*(K*P-O*L)
      P2=(C*E-A*G)*(J*P-N*L)
      P3=(A*H-D*E)*(J*O-N*K)
      P4=(B*G-C*F)*(I*P-M*L)
      P5=(C*H-D*G)*(I*N-M*J)
      P6=(D*F-B*H)*(I*O-M*K)
C
```

```
      R=P1+P2+P3+P4+P5+P6
C
      RETURN
      END
```

```
      PROGRAM FBCC (INPUT,OUTPUT)
C
C
C
C CHADI-COHEN EXTRAPOLATED ON FOUR POINTS,
C FOR BODY CENTERED LATTICE
C
C CALCULATES THE "F(1)"
C
      DIMENSION C(2000),G(4),X(4),DN(4,4),DD(4,4)
10    CONTINUE
      PI=3.141592654
      DO 101 IJ=1,4,1
      G(IJ)=0.0
101   CONTINUE
      NSTART=3
C     READ *,NSTART
C NSTART IS THE STARTING ORDER
      READ *,F
      IF (F-1.1E+9)15,20,20
15    DO 102 III=1,4,1
      NU=NSTART+III-1
      LIM=2*(2**NU)
      TH=2*PI/LIM
      LIMD=LIM-1
      DO 6 M=1,LIMD,2
      C(M)=COS(TH*M/2.00)
      C(M+1)=COS(TH*M)
6     CONTINUE
      CALL CALBCC(LIMD,NU,C,F,G1,IPTS)
      G(III)=G1
      X(III)=1.0/(LIM*1.0)
102   CONTINUE
      DO 105 LL=1,4,1
      DN(LL,1)=X(LL)**3
      DD(LL,1)=DN(LL,1)
      DN(LL,2)=X(LL)*X(LL)
      DD(LL,2)=DN(LL,2)
      DN(LL,3)=X(LL)
      DD(LL,3)=X(LL)
      DN(LL,4)=G(LL)
      DD(LL,4)=1.0
105   CONTINUE
      CALL DET4(DN,RN)
      CALL DET4(DD,RD)
      FF1=RN/RD
      T2=0.25*(1.0-(1.0/FF1))
      PRINT *,F,FF1,T2
      GO TO 10
20    CONTINUE
```

```
      END
      SUBROUTINE DET4(DD,R)
C CALCULATES A 4*4 DETERMINANT
C SENDS THE RESULTS BACK IN R
      REAL I,J,K,L,M,N
      DIMENSION DD(4,4)
C
      A=DD(1,1)
      B=DD(1,2)
      C=DD(1,3)
      D=DD(1,4)
C
      E=DD(2,1)
      F=DD(2,2)
      G=DD(2,3)
      H=DD(2,4)
C
      I=DD(3,1)
      J=DD(3,2)
      K=DD(3,3)
      L=DD(3,4)
C
      M=DD(4,1)
      N=DD(4,2)
      O=DD(4,3)
      P=DD(4,4)
C
      P1=(A*F-B*E)*(K*P-O*L)
      P2=(C*E-A*G)*(J*P-N*L)
      P3=(A*H-D*E)*(J*O-N*K)
      P4=(B*G-C*F)*(I*P-M*L)
      P5=(C*H-D*G)*(I*N-M*J)
      P6=(D*F-B*H)*(I*O-M*K)
C
      R=P1+P2+P3+P4+P5+P6
C
      RETURN
      END
      SUBROUTINE CALBCC(LIMD,N,C,F,FF,IPTS)
C CALCULATES THE "GREEN'S FUNCTION INCLUDING
C THE SECOND NEIGHBOURS FOR BODY CENTERED
C LATTICE
C
      DIMENSION C(2000)
      IPTS=0
C IPTS IS A COUNTER OF POINTS AT WHICH THE
C FUNCTION IS EFFECTIVELY CALCULATED
      SU=0.0
      NPO=2*(8**(N-1))
      LIM=LIMD+1
```

```
      DE=4.0+3.0*F
      DO 1 IX=1,LIMD,2
      CX2=C(IX)
      CX=C(IX+1)
      DO 1 IY=1,IX,2
      CY2=C(IY)
      CY=C(IY+1)
      DO 1 IZ=1,IY,2
      CZ2=C(IZ)
      CZ=C(IZ+1)
      IF (IX+IY-LIM) 2,3,1
2     AL=6.0
      IF ((IX.EQ.IY).AND.(IY.EQ.IZ)) GO TO 4
      IF (IX.EQ.IY) GO TO 5
      IF (IX.EQ.IZ) GO TO 5
      IF (IY.EQ.IZ) GO TO 5
      GO TO 6
4     AL=1.0
      GO TO 6
5     AL=3.0
      GO TO 6
3     AL=3.0
      IF (IX.EQ.IY) GO TO 7
      IF (IX.EQ.IZ) GO TO 7
      IF (IY.EQ.IZ) GO TO 7
      GO TO 6
7     AL=1.0
6     CONTINUE
      IPTS=IPTS+1
      AA=4.0*CX2*CY2*CZ2
      BB=F*(CX+CY+CZ)
      RJJ=(AA+BB)/DE
      TE=AL/(1.0-RJJ)
      SU=SU+TE
1     CONTINUE
      FF=SU/(NPO*1.0)
      RETURN
      END
C
```

```
      PROGRAM FFCC(INPUT,OUTPUT)
C
C
C  CHADI-COHEN PROCEDURE EXTRAPOLATED ON 4 POINTS
C TO CALCULATE THE GREEN'S FUNCTION FOR THE
C  FCC LATTICE
C
      DIMENSION C(2000),G(4),X(4)
C
10    CONTINUE
      PI=3.141592654
      NSTART=3
C NSTART IS STARTING ORDER HERE
      READ *,F
      IF (F-1.1E+9) 15,20,20
15    DO 1 I=1,4,1
      G(I)=0.0
      X(I)=0.0
1     CONTINUE
      DO 2 I=1,4,1
      N=NSTART+I-1
      LIM=2*(2**N)
      TH=(2.0*PI)/(LIM*1.0)
      LIMD=LIM-1
      NU=0
      DO 3 M=1,LIMD,2
      C(M)=COS(TH*M/2.00)
      C(M+1)=COS(TH*M)
3     CONTINUE
      CALL CALC(LIMD,NU,C,F,G(I))
      X(I)=1.0/LIM
2     CONTINUE
      X1=X(1)
      X2=X(2)
      X3=X(3)
      X4=X(4)
      X12=X1*X1
      X22=X2*X2
      X32=X3*X3
      X42=X4*X4
      X13=X12*X1
      X23=X22*X2
      X33=X32*X3
      X43=X42*X4
      CALL DET4(X13,X12,X1,1.0,X23,X22,X2,1.0,X33,X32,X3,1.0,
     1X43,X42,X4,1.0,DETDEN)
      CALL DET4(X13,X12,X1,G(1),X23,X22,X2,G(2),X33,X32,X3,G(3),
     1X43,X42,X4,G(4),DETNUM)
      GF=DETNUM/DETDEN
      T2=0.25*(1.0-(1.0/GF))
```

```
      PRINT *,F,GF,T2
      GO TO 10
20    CONTINUE
      END
      SUBROUTINE DET4(A,B,C,D,E,F,G,H,I,J,K,L,M,N,O,P,R)
      REAL I,J,K,L,M,N
      P1=(A*F-B*E)*(K*P-O*L)
      P2=(C*E-A*G)*(J*P-N*L)
      P3=(A*H-D*E)*(J*O-N*K)
      P4=(B*G-C*F)*(I*P-M*L)
      P5=(C*H-D*G)*(I*N-M*J)
      P6=(D*F-B*H)*(I*O-M*K)
      R=P1+P2+P3+P4+P5+P6
      RETURN
      END
      SUBROUTINE CALC(LIMD,NU,C,F,FF)
      DIMENSION C(2000)
      INTEGER OJ
      SU=0.0
      NU=0
C NU IS THE TOTAL NUMBER OF POINTS IN
C THE ORDER UNDER CONSIDERATION;
C IT IS EQUAL TO LIM
      LIM=LIMD+1
      DE=6.0+3.0*F
      DO 1 IX=1,LIMD,2
      CX2=C(IX)
C CX2 IS THE "HALF-ANGLE"
      CX=C(IX+1)
      DO 1 IY=1,IX,2
      CY2=C(IY)
      CY=C(IY+1)
      DO 1 IZ=1,IY,2
      CZ2=C(IZ)
      CZ=C(IZ+1)
      IF ((IX+IY+IZ)-(3*LIM/2)) 10,10,1
10    CONTINUE
      OJ=6
      IF((IX.EQ.IY).AND.(IY.EQ.IZ)) GO TO 2
      IF((IX.EQ.IY).OR.(IX.EQ.IZ).OR.(IY.EQ.IZ)) GO TO 3
      GO TO 4
2     OJ=1
      GO TO 4
3     OJ=3
4     NU=NU+OJ
      AA=(CX2*CY2+CX2*CZ2+CY2*CZ2)*2.0
      BB=(CX+CY+CZ)*F
      RJJ=(AA+BB)/DE
      TE=OJ/(1.0-RJJ)
      SU=SU+TE
```

```
1     CONTINUE
      FF=SU/NU
      RETURN
      END
```

```
      PROGRAM T2SC (INPUT,OUTPUT)
C
C
      INTEGER Z1,Z2
      DIMENSION C(3000),G(4),X(4)
      DIMENSION H(4)
      DIMENSION D(4,4)
C
C
      JK=1
      Z1=6
      Z2=12
      PI=3.141592654
      DO 11 I=1,3,1
      G(I)=0.0
      H(I)=0.0
11    CONTINUE
      PRINT 199
      PRINT 199
      PRINT 200
200   FORMAT (3X,1HF,10X,3HT2D,8X,3HT2P,8X,4HT2NR,7X,4HT2NX
     1,7X,3HP11,8X,3HP22,8X,1HX,10X,1HY)
199   FORMAT (1H )
      PRINT 199
101   CONTINUE
      READ *,F,F1,T2
      JK=JK+1
      IF(F.GE.(2.E08)) GO TO 100
C
C
      DO 15 NN=1,4,1
      N=NN+1
C STARTING ORDER IS FIXED HERE
      TH=PI/(4.0*(2.0**N))
      LI=(4*(2**N))-1
      DO 6 M=1,LI,2
      C(M)=COS(TH*M)
6     CONTINUE
      X(NN)=1.0/((LI+1)*1.0)
      CALL CALC(LI,C,F,F1,GG,HH)
      G(NN)=GG
      H(NN)=HH
15    CONTINUE
      DO 69 I=1,4,1
      DO 69 K=1,3,1
      D(I,K)=X(I)**(4-K)
69    CONTINUE
      DO 70 K=1,4,1
      D(K,4)=G(K)
70    CONTINUE
```

```
      CALL DET4 (D,DETNUM)
      DO 71 K=1,4,1
      D(K,4)=1.0
71    CONTINUE
      CALL DET4(D,DETDEN)
      T2NR=DETNUM/DETDEN
      DO 72 K=1,4,1
      D(K,4)=H(K)
72    CONTINUE
      CALL DET4(D,DETNUM)
      T2NX=DETNUM/DETDEN
      P11=(T2NR*Z1-0.25)/((Z1-1)*1.0)
      P22=(T2NX*Z2-0.25)/((Z2-1)*1.0)
      Q11=2.0*SQRT(ABS(P11))
      Q22=2.0*SQRT(ABS(P22))
      T2D=0.25*(1.0-(1.0/F1))
      T2PA=0.25*Z1+Z1*(Z1-1)*P11
      T2PB=(0.25*Z2+Z2*(Z2-1)*P22)*F*F
      T2PC=2.0*Z1*Z2*SQRT(ABS(P11*P22))*F
      T2PD=Z1*Z1+2*Z1*Z2*F+Z2*Z2*F*F
      T2P=(T2PA+T2PB+T2PC)/T2PD
      PRINT 201,F,T2D,T2P,T2NR,T2NX,P11,P22
201   FORMAT (G9.2,2X,8(F9.6,2X))
      IF((INT(JK/5.0)).EQ.(JK/5.0)) PRINT 199
      GO TO 101
100   CONTINUE
      END
      SUBROUTINE CALC(LI,C,F,F1,G,H)
      DIMENSION C(3000)
      REAL NU
      REAL J1Q,J2Q
      SUG=0.0
      SUH=0.0
      NU=0.0
      DE=3.0+6.0*F
      DO 1 I=1,LI,2
      CI=C(I)
      DO 1 J=1,I,2
      CJ=C(J)
      DO 1 K=1,J,2
      CK=C(K)
      IF((I.EQ.J).AND.(I.EQ.K).AND.(J.EQ.K)) GO TO 2
      IF((I.EQ.J).OR.(I.EQ.K).OR.(J.EQ.K)) GO TO 3
      AL=6.0
      GO TO 4
2     AL=1.0
      GO TO 4
3     AL=3.0
4     CONTINUE
      AA=CI+CJ+CK
```

```
      BB=2.0*F*((CI*CJ)+(CI*CK)+(CJ*CK))
      RJJ=(AA+BB)/DE
      CFQ=1.0/(F1*4.0*(1.0-RJJ))
      NU=NU+AL
      J1Q=AA/3.0
      J2Q=BB/(6.0*F)
C
C
C
      TE1=J1Q*J1Q*CFQ*AL
      TE2=J2Q*J2Q*CFQ*AL
      SUG=SUG+TE1
      SUH=SUH+TE2
1     CONTINUE
      G=SUG/NU
      H=SUH/NU
      RETURN
      END
      SUBROUTINE DET4(DD,R)
      REAL I,J,K,L,M,N
      DIMENSION DD(4,4)
C
      A=DD(1,1)
      B=DD(1,2)
      C=DD(1,3)
      D=DD(1,4)
C
      E=DD(2,1)
      F=DD(2,2)
      G=DD(2,3)
      H=DD(2,4)
C
      I=DD(3,1)
      J=DD(3,2)
      K=DD(3,3)
      L=DD(3,4)
C
      M=DD(4,1)
      N=DD(4,2)
      O=DD(4,3)
      P=DD(4,4)
C
      P1=(A*F-B*E)*(K*P-O*L)
      P2=(C*E-A*G)*(J*P-N*L)
      P3=(A*H-D*E)*(J*O-N*K)
      P4=(B*G-C*F)*(I*P-M*L)
      P5=(C*H-D*G)*(I*N-M*J)
      P6=(D*F-B*H)*(I*O-M*K)
C
      R=P1+P2+P3+P4+P5+P6
```

```
C
      RETURN
      END
```

```
      PROGRAM T2BCC (INPUT,OUTPUT)
C
C
C
C
      INTEGER Z1,Z2
      DIMENSION C(3000),G(4),X(4)
      DIMENSION H(4),D(4,4)
      Z1=8
      Z2=6
      PI=3.141592654
      DO 11 I=1,4,1
      G(I)=0.0
      H(I)=0.0
11    CONTINUE
      PRINT 199
      PRINT 210
210   FORMAT (25X,3HBCC)
      PRINT 199
      PRINT 200
200   FORMAT (3X,1HF,10X,3HT2D,8X,3HT2P,8X,4HT2NR,7X,4HT2NX
     1,7X,3HP11,8X,3HP22)
199   FORMAT (1H )
      PRINT 199
101   CONTINUE
      J=1
2222  CONTINUE
      READ *,F,GF,TTT
      J=J+1
      IF(F-1.1E+8) 99,100,100
99    CONTINUE
      DO 15 NN=1,4,1
      N=NN+3
      LIM=2**N
      LIMD=LIM-1
      TH=2.0*PI/LIM
      DO 6 M=1,LIMD,2
      C(M)=COS(TH*M/2.0)
      C(M+1)=COS(TH*M)
6     CONTINUE
      X(NN)=1.0/(LIM*1.0)
      CALL CALBCC(LIM,C,F,GF,GG,HH)
      G(NN)=GG
      H(NN)=HH
15    CONTINUE
      DO 69 I=1,4,1
      DO 69 K=1,3,1
      D(I,K)=X(I)**(4-K)
69    CONTINUE
      DO 70 K=1,4,1
```

```
      D(K,4)=G(K)
70    CONTINUE
      CALL DET4(D,DETNUM)
      DO 71 K=1,4,1
      D(K,4)=1
71    CONTINUE
      CALL DET4(D,DETDEN)
      T2NR=DETNUM/DETDEN
      DO 72 K=1,4,1
      D(K,4)=H(K)
72    CONTINUE
      CALL DET4(D,DETNUM)
      T2NX=DETNUM/DETDEN
      P11=(T2NR*Z1-0.25)/((Z1-1)*1.0)
      P22=(T2NX*Z2-0.25)/((Z2-1)*1.0)
      Q11=2.0*SQRT(ABS(P11))
      Q22=2.0*SQRT(ABS(P22))
      T2D=0.25*(1.0-(1.0/GF))
      T2PA=0.25*Z1+Z1*(Z1-1)*P11
      T2PB=(0.25*Z2+Z2*(Z2-1)*P22)*F*F
      T2PC=2.0*Z1*Z2*SQRT(ABS(P11*P22))*F
      T2PD=Z1*Z1+2*Z1*Z2*F+Z2*Z2*F*F
      T2P=(T2PA+T2PB+T2PC)/T2PD
      PRINT 201,F,T2D,T2P,T2NR,T2NX,P11,P22
201   FORMAT (G9.2,2X,6(F9.6,2X))
      IF((INT(J/5.0)).EQ.(J/5.0)) PRINT 199
      GO TO 2222
100   CONTINUE
      END
      SUBROUTINE CALBCC(LIM,C,F,GF,G,H)
      DIMENSION  (3000)
      REAL NU
      REAL J1Q,J2Q
      SUG=0.0
      SUH=0.0
      NU=0.0
      DE=4.0+3.0*F
      LIMD=LIM-1
      DO 1 IX=1,LIMD,2
      CX2=C(IX)
      CX=C(IX+1)
      DO 1 IY=1,IX,2
      CY2=C(IY)
      CY=C(IY+1)
      DO 1 IZ=1,IY,2
      CZ2=C(IZ)
      CZ=C(IZ+1)
      IF (IX+IY-LIM) 2,3,1
2     AL=6.0
      IF ((IX.EQ.IY).AND.(IY.EQ.IZ)) GO TO 4
```

```
      IF (IX.EQ.IY) GO TO 5
      IF (IX.EQ.IZ) GO TO 5
      IF (IY.EQ.IZ) GO TO 5
      GO TO 6
4     AL=1.0
      GO TO 6
5     AL=3.0
      GO TO 6
3     AL=3.0
      IF(IX.EQ.IY) GO TO 7
      IF (IX.EQ.IZ) GO TO 7
      IF (IY.EQ.IZ) GO TO 7
      GO TO 6
7     AL=1.0
6     CONTINUE
      AA=4.0*CX2*CY2*CZ2
      BB=F*(CX+CY+CZ)
      RJJ=(AA+BB)/DE
      CFQ=1.0/(GF*4.0*(1.0-RJJ))
      NU=NU+AL
      J1Q=AA/4.0
      J2Q=BB/(3.0*F)
C ACTUALLY THESE ARE THE J(Q)/J(0)
      TE1=J1Q*J1Q*CFQ*AL
      TE2=J2Q*J2Q*CFQ*AL
      SUG=SUG+TE1
      SUH=SUH+TE2
1     CONTINUE
      G=SUG/NU
      H=SUH/NU
      RETURN
      END
      SUBROUTINE DET4(DD,R)
C CALCULATES A 4X4 DETERMINANT
C SENDS THE RESULT IN R
      REAL I,J,K,L,M,N
      DIMENSION DD(4,4)
C
      A=DD(1,1)
      B=DD(1,2)
      C=DD(1,3)
      D=DD(1,4)
C
      E=DD(2,1)
      F=DD(2,2)
      G=DD(2,3)
      H=DD(2,4)
C
      I=DD(3,1)
      J=DD(3,2)
```

```
      K=DD(3,3)
      L=DD(3,4)
C
      M=DD(4,1)
      N=DD(4,2)
      O=DD(4,3)
      P=DD(4,4)
C
      P1=(A*F-B*E)*(K*P-O*L)
      P2=(C*E-A*G)*(J*P-N*L)
      P3=(A*H-D*E)*(J*O-N*K)
      P4=(B*G-C*F)*(I*P-M*L)
      P5=(C*H-D*G)*(I*N-M*J)
      P6=(D*F-B*H)*(I*O-M*K)
C
      R=P1+P2+P3+P4+P5+P6
C
      RETURN
      END
```

```
      PROGRAM T2FCC(INPUT,OUTPUT)
      INTEGER Z1,Z2
      DIMENSION C(3000),G(4),X(4)
      DIMENSION H(4)
      DIMENSION D(4,4)
      Z1=12
      Z2=6
      PI=3.141592654
      PRINT 199
      PRINT 210
      J=1
210   FORMAT (25X,3HFCC)
      PRINT 199
      PRINT 200
200   FORMAT(3X,1HF,10X,3HT2D,8X,3HT2P,8X,4HT2NR,7X,4HT2NX
     1,7X,3HP11,8X,3HP22)
199   FORMAT (1H )
      PRINT 199
101   CONTINUE
1000  CONTINUE
      READ *,F,GF,T2
      J=J+1
      IF (F.GT.(1E08)) GO TO 1001
      DO 15 NN=1,4,1
      N=NN+3
      LIM=2**N
      LIMD=LIM-1
      TH=2.0*PI/LIM
      NU=0
      DO 6 M=1,LIMD,2
      C(M)=COS(TH*M/2.0)
      C(M+1)=COS(TH*M)
6     CONTINUE
      X(NN)=1.0/(LIM*1.0)
      CALL CALFCC(LIM,C,F,GF,GG,HH)
      G(NN)=GG
      H(NN)=HH
15    CONTINUE
      DO 69 I=1,4,1
      DO 69 K=1,3,1
      D(I,K)=X(I)**(4-K)
69    CONTINUE
      DO 70 K=1,4,1
      D(K,4)=G(K)
70    CONTINUE
      CALL DET4(D,DETNUM)
      DO 71 K=1,4,1
      D(K,4)=1
71    CONTINUE
      CALL DET4(D,DETDEN)
```

```
      T2NR=DETNUM/DETDEN
      DO 72 K=1,4,1
      D(K,4)=H(K)
72    CONTINUE
      CALL DET4 (D,DETNUM)
      T2NX=DETNUM/DETDEN
      P11=(T2NR*Z1-0.25)/((Z1-1)*1.0)
      P22=(T2NX*Z2-0.25)/((Z2-1)*1.0)
      Q11=2.0*SQRT(ABS(P11))
      Q22=2.0*SQRT(ABS(P22))
      T2D=0.25*(1.0-(1.0/GF))
      T2PA=0.25*Z1+Z1*(Z1-1)*P11
      T2PB=(0.25*Z2+Z2*(Z2-1)*P22)*F*F
      T2PC=2.0*Z1*Z2*SQRT(ABS(P11*P22))*F
      T2PD=Z1*Z1+2*Z1*Z2*F+Z2*Z2*F*F
      T2P=(T2PA+T2PB+T2PC)/T2PD
      PRINT 201,F,T2D,T2P,T2NR,T2NX,P11,P22
201   FORMAT (G9.2,2X,6(F9.6,2X))
      IF((INT(J/5.0)).EQ.(J/5.0)) PRINT 199
100   CONTINUE
      GO TO 1000
1001  CONTINUE
      END
      SUBROUTINE CALFCC(LIM,C,F,GF,G,H)
      DIMENSION C(3000)
      REAL NU
      REAL J1Q,J2Q
      SUG=0.0
      SUH=0.0
      NU=0.0
      DE=6.0+3.0*F
      LIMD=LIM-1
      DO 1 IX=1,LIMD,2
      CX2=C(IX)
      CX=C(IX+1)
      DO 1 IY=1,IX,2
      CY2=C(IY)
      CY=C(IY+1)
      DO 1 IZ=1,IY,2
      CZ2=C(IZ)
      CZ=C(IZ+1)
      IF((IX+IY+IZ)-(3*LIM/2)) 10,10,1
10    CONTINUE
      OJ=6.0
      IF((IX.EQ.IY).AND.(IY.EQ.IZ)) GO TO 2
      IF((IX.EQ.IY).OR.(IX.EQ.IZ).OR.(IY.EQ.IZ)) GO TO 3
      GO TO 4
2     OJ=1.0
      GO TO 4
3     OJ=3.0
```

```
4       NU=NU+OJ
        AA=(CX2*CY2+CX2*CZ2+CY2*CZ2)*2.0
        BB=(CX+CY+CZ)*F
        RJJ=(AA+BB)/DE
        CFQ=1.0/(GF*4.0*(1.0-RJJ))
        J1Q=AA/6.0
        J2Q=BB/(3.0*F)
        CFQOJ=CFQ*OJ
        TE1=J1Q*J1Q*CFQOJ
        TE2=J2Q*J2Q*CFQOJ
        SUG=SUG+TE1
        SUH=SUH+TE2
1       CONTINUE
        G=SUG/NU
        H=SUH/NU
        RETURN
        END
        SUBROUTINE DET4(DD,R)
        REAL I,J,K,L,M,N
        DIMENSION DD(4,4)
C
        A=DD(1,1)
        B=DD(1,2)
        C=DD(1,3)
        D=DD(1,4)
C
        E=DD(2,1)
        F=DD(2,2)
        G=DD(2,3)
        H=DD(2,4)
C
        I=DD(3,1)
        J=DD(3,2)
        K=DD(3,3)
        L=DD(3,4)
C
        M=DD(4,1)
        N=DD(4,2)
        O=DD(4,3)
        P=DD(4,4)
C
        P1=(A*F-B*E)*(K*P-O*L)
        P2=(C*E-A*G)*(J*P-N*L)
        P3=(A*H-D*E)*(J*O-N*K)
        P4=(B*G-C*F)*(I*P-M*L)
        P5=(C*H-D*G)*(I*N-M*J)
        P6=(D*F-B*H)*(I*O-M*K)
C
        R=P1+P2+P3+P4+P5+P6
C       RETURN
        END
```

```
      PROGRAM BETAC(INPUT,OUTPUT)
C
C
      INTEGER Z1,FZ1,Z2,FZ2
      I=1
      PRINT *,1H
      PRINT *,7H        ,3HA=1
      PRINT *,1H
      Z1=12
      Z2=6
C SC: Z1=6, Z2=12
C BCC: Z1=8, Z2=6
C FCC: Z1=12,Z2=6
      IF (Z1.EQ.6) PRINT *,7H        ,2HSC
      IF (Z1.EQ.8) PRINT *,7H        ,3HBCC
      IF (Z1.EQ.12) PRINT *,7H       ,3HFCC
      PRINT *,1H
      PRINT 640
640   FORMAT(13X,1HF,13X,4HBETA,7X,6H1/BETA,11X,3HP11,11X,3HP22
     1,11X,3HQ11,11X,3HQ22)
      PRINT *,1H
C
      BETA=1.00
999   CONTINUE
      READ *,F,T2D,T2P,T2NR,T2NX,P11,P22
      I=I+1
      IF(F.GE.(3.1E04)) GO TO 1
      PREB=0.00001
      FZ1=0
      FZ2=0
      RI=0.0
      RJ=0.0
      RESI=0.0
      RESJ=0.0
      CALL FACT(Z1,FZ1)
      CALL FACT(Z2,FZ2)
      Q11=2.0*SQRT(P11)
      Q22=2.0*SQRT(P22)
      F2=F*F
C NEWTON-RAPHSON FOR BETA STARTS HERE
150   CONTINUE
      BI=BETA
      BJ=BETA/2.0
165   CALL FUNB(BJ,Z1,Z2,FZ1,FZ2,F,Q11,Q22,RJ)
171   CALL FUNB(BI,Z1,Z2,FZ1,FZ2,F,Q11,Q22,RI)
      IF((ABS(BJ-BI))-PREB) 160,161,161
161   RK=(RJ-RI)/(BJ-BI)
      BJ=BI
      BI=BI-RI/RK
      RJ=RI
```

```
C NEW RJ=OLD RI AND THEN CALCULATE THE NEW RI
C BY "GO TO 171"
      GO TO 171
160   BETA=BI
      REI=I*1.00
      IF(INT(REI/5.0)-(REI/5.0)) 641,643,641
643   PRINT *,1H
641   RINV=1.00/BETA
      PRINT 642,F,BETA,RINV,P11,P22,Q11,Q22
642   FORMAT (10X,G9.2,4X,6(F9.6,5X))
      GO TO 999
1     CONTINUE
      PRINT *,1H
      PRINT *,1H
      PRINT *,1H
      STOP
      END
      SUBROUTINE FUNB(BK,Z1,Z2,FZ1,FZ2,F,Q11,Q22,RR)
      INTEGER FLA,FLAZ1,FMU,FMUZ2,FZ1,FZ2
      INTEGER Z1,Z2
      SIGMA=0.0
      LZ1=Z1+1
      DO 500 LLA=1,LZ1,1
      LA=LLA-1
      CALL FACT(LA,FLA)
      LAZ1=Z1-LA
      CALL FACT(LAZ1,FLAZ1)
      LZ2=Z2+1
      DO 500 LMU=1,LZ2,1
      MU=LMU-1
      CLAMU=Z1*1.0-2.0*LA+F*(Z2-2*MU)
      CALL FACT(MU,FMU)
      MUZ2=Z2-MU
      CALL FACT(MUZ2,FMUZ2)
      CLAZ1=FZ1/(FLAZ1*FLA)
      CMUZ2=FZ2/(FMUZ2*FMU)
      PAR1=(1.0-Q11)**LAZ1
      PAR2=(1.0+Q11)**LA
      PAR3=(1.0-Q22)**MUZ2
      PAR4=(1.0+Q22)**MU
      QLAMU=CLAZ1*CMUZ2*PAR1*PAR2*PAR3*PAR4
      X=0.25*BK*CLAMU
      IF (ABS(X)-650)510,520,520
      RETURN
520   PRINT *,5HFUNB.
510   XA=EXP(X)
      XB=EXP(-1.0*X)
      THX=(XA-XB)/(XA+XB)
      TERM=QLAMU*THX*(THX-(CLAMU/(Z1+(F*Z2))))
      SIGMA=SIGMA+TERM
```

```
500   CONTINUE
      RR=SIGMA
      RETURN
      END
      SUBROUTINE FACT(NN,FACTN)
      INTEGER FACTN
C TABLE OF FACTORIALS NEEDED
      IF (NN) 1,1,13
13    CONTINUE
      GO TO (1,2,3,4,5,6,7,8,9,10,11,12) NN
1     FACTN=1
      RETURN
2     FACTN=2
      RETURN
3     FACTN=6
      RETURN
4     FACTN=24
      RETURN
5     FACTN=120
      RETURN
6     FACTN=720
      RETURN
7     FACTN=5040
      RETURN
8     FACTN=40320
      RETURN
9     FACTN=362880
      RETURN
10    FACTN=3628800
      RETURN
11    FACTN=39916800
      RETURN
12    FACTN=479001600
      RETURN
      END
```

```
      PROGRAM BETACP(INPUT,OUTPUT)
C
C  CALCULATES BETA CRITICAL AFTER P11 AND P22;
C WITH A'=1 RATHER THAN A=1.
C THE ALGORITHM IS "NEWTON-RAPHSON-SECANT"
C
C
      INTEGER Z1,FZ1,Z2,FZ2
      I=1
      PRINT *,1H
      PRINT *,7H       ,4HA'=1
      PRINT *,1H
      Z1=12
      Z2=6
C SC: Z1=6, Z2=12
C BCC: Z1=8, Z2=6
C FCC: Z1=12, Z2=6
      IF (Z1.EQ.6) PRINT *,7H        ,2HSC
      IF (Z1.EQ.8) PRINT *,7H        ,3HBCC
      IF (Z1.EQ.12) PRINT *,7H        ,3HFCC
      PRINT *,1H
      PRINT 640
640   FORMAT(13X,1HF,13X,4HBETA,7X,6H1/BETA,11X,3HP11,11X,3HP22
     1,11X,3HQ11,11X,3HQ22)
      PRINT *,1H
      BETA=1.00
999   CONTINUE
      READ *,F,T2D,T2P,T2NR,T2NX,P11,P22
      I=I+1
      IF(F.GE.(3.1E04)) GO TO 1
C
C REQUIRED PRECISION FOR THE NEWTON RAPHSON,  IS SET HERE
      PREB=0.00001
      FZ1=0
      FZ2=0
      RI=0.0
      RJ=0.0
      RESI=0.0
      RESJ=0.0
      CALL FACT(Z1,FZ1)
      CALL FACT(Z2,FZ2)
      Q11=2.0*SQRT(P11)
      Q22=2.0*SQRT(P22)
      F2=F*F
C NEWTON-RAPHSON FOR BETA STARTS HERE
150   CONTINUE
      BI=BETA
      BJ=BETA/2.0
165   CALL FUNB(BJ,Z1,Z2,FZ1,FZ2,F,Q11,Q22,RJ)
171   CALL FUNB(BI,Z1,Z2,FZ1,FZ2,F,Q11,Q22,RI)
```

```
      IF((ABS(BJ-BI))-PREB) 160,161,161
161   RK=(RJ-RI)/(BJ-BI)
      BJ=BI
      BI=BI-RI/RK
      RJ=RI
C NEW RJ=OLD RI AND THEN CALCULATE THE NEW RI
C BY "GO TO 171"
      GO TO 171
160   BETA=BI
      REI=I*1.00
      IF(INT(REI/5.0)-(REI/5.0)) 641,643,641
643   PRINT *,1H
641   RINV=1.00/BETA
      PRINT 642,F,BETA,RINV,P11,P22,Q11,Q22
642   FORMAT (10X,G9.2,4X,6(F9.6,5X))
      GO TO 999
1     CONTINUE
      PRINT *,1H
      PRINT *,1H
      PRINT *,1H
      STOP
      END
      SUBROUTINE FUNB(BK,Z1,Z2,FZ1,FZ2,F,Q11,Q22,RR)
      INTEGER FLA,FLAZ1,FMU,FMUZ2,FZ1,FZ2
      INTEGER Z1,Z2
      SIGMA=0.0
      LZ1=Z1+1
      DO 500 LLA=1,LZ1,1
      LA=LLA-1
      CALL FACT(LA,FLA)
      LAZ1=Z1-LA
      CALL FACT(LAZ1,FLAZ1)
      LZ2=Z2+1
      DO 500 LMU=1,LZ2,1
      MU=LMU-1
      CLAMU=Z1*1.0-2.0*LA+F*(Z2-2*MU)
      CALL FACT(MU,FMU)
      MUZ2=Z2-MU
      CALL FACT(MUZ2,FMUZ2)
      CLAZ1=FZ1/(FLAZ1*FLA)
      CMUZ2=FZ2/(FMUZ2*FMU)
      PAR1=(1.0-Q11)**LAZ1
      PAR2=(1.0+Q11)**LA
      PAR3=(1.0-Q22)**MUZ2
      PAR4=(1.0+Q22)**MU
      QLAMU=CLAZ1*CMUZ2*PAR1*PAR2*PAR3*PAR4
      X=0.25*BK*CLAMU
      XA=EXP(X)
      XB=EXP(-1.0*X)
      THX=(XA-XB)/(XA+XB)
```

```
      TERM=QLAMU*CLAMU*(THX-(CLAMU/(Z1+F*Z2)))
      SIGMA=SIGMA+TERM
500   CONTINUE
      RR=SIGMA
      RETURN
      END
      SUBROUTINE FACT(NN,FACTN)
      INTEGER FACTN
C TABLE OF FACTORIALS NEEDED
      IF (NN) 1,1,13
13    CONTINUE
      GO TO (1,2,3,4,5,6,7,8,9,10,11,12) NN
1     FACTN=1
      RETURN
2     FACTN=2
      RETURN
3     FACTN=6
      RETURN
4     FACTN=24
      RETURN
5     FACTN=120
      RETURN
6     FACTN=720
      RETURN
7     FACTN=5040
      RETURN
8     FACTN=40320
      RETURN
9     FACTN=362880
      RETURN
10    FACTN=3628800
      RETURN
11    FACTN=39916800
      RETURN
12    FACTN=479001600
      RETURN
      STOP
      END
```

```
      PROGRAM REGRE(INPUT,OUTPUT)
      REAL INTER
C
C LINEAR AND QUADRATIC REGRESSION
C
C
      DIMENSION X(200),Y(200)
      I=0
C
1     CONTINUE
      I=I+1
10    CONTINUE
      READ *,ENN,TCF
      IF(ENN-900000) 15,5,5
15    CONTINUE
      IF(ENN-18) 10,10,20
C GREATER THAN F=1 VALUES ONLY
C 10,10,20
20    X(I)=TCF
      Y(I)=ENN
      GO TO 1
5     CONTINUE
      NB=I-1
      PRINT *,3HNB=,NB
      SX1=0.0
      SX2=0.0
      SX3=0.0
      SX4=0.0
      SXY=0.0
      SX2Y=0.0
      SY=0.0
      DO 2 J=1,NB,1
      A=X(J)
      A2=A*A
      A3=A2*A
      A4=A3*A
      SX1=SX1+A
      SX2=SX2+A2
      SX3=SX3+A3
      SX4=SX4+A4
      B=Y(J)
      SXY=SXY+A*B
      SX2Y=SX2Y+A2*B
      SY=SY+B
2     CONTINUE
      D1=NB*(SX2*SX4-SX3*SX3)
      D2=SX1*(SX2*SX3-SX1*SX4)
      D3=SX2*(SX1*SX3-SX2*SX2)
      D=D1+D2+D3
      CC1=NB*(SX2*SX2Y-SX3*SXY)
```

```
      CC2=SX1*(SX1*SX2Y-SX2*SXY)
      CC3=SY*(SX1*SX3-SX2*SX2)
      AA2=(CC1-CC2+CC3)/D
      CN=SY-AA2*SX2
      CM=SXY-AA2*SX3
      AA1=(NB*CM-CN*SX1)/(NB*SX2-SX1*SX1)
      AA0=(CN-AA1*SX1)/NB
      PRINT 99
99    FORMAT (1H )
      PRINT 99
      PRINT *,5H      ,9HQUADRATIC
      PRINT 99
      PRINT *,3HA0=,AA0
      PRINT *,3HA1=,AA1
      PRINT *,3HA2=,AA2
      PRINT 99
      PRINT *,5H      ,6HLINEAR
      PRINT *,5H      ,8HINVERTED
      PRINT 99
      CN=SY
      CM=SXY
      AA1=(NB*CM-CN*SX1)/(NB*SX2-SX1*SX1)
      AA0=(CN-AA1*SX1)/NB
      SLOPE=1/AA1
      INTER=AA0/AA1
      PRINT *,6HSLOPE=,SLOPE
      PRINT *,10HINTERCEPT=,INTER
      END
```